Pacific Northwest NATIONAL LABORATORY

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In a report published in *Chemical Reviews*, PNNL researchers say future batteries used by the energy grid to store power from the wind and the sun must be reliable, durable and safe, but affordability is key to widespread market deployment.

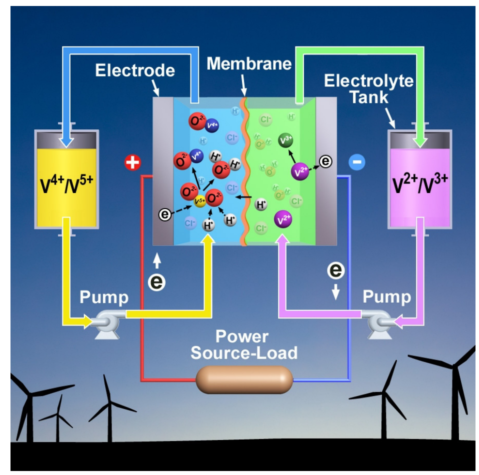
U.S. DEPARTMENT OF ENERGY

Transformational Materials Science Initiative

Revolutionizing Materials for Energy Storage

The Transformational Materials Science Initiative at Pacific Northwest National Laboratory is elucidating the principles of synthesizing and assembling functional nanostructures, understanding nanoscale-to-macroscale phenomena within materials of interest, and developing multi-scale computational models and unique characterization tools to understand essential phenomena in energy storage materials. Chief among PNNL's achievements in the Transformational Materials Science Initiative are

- **Designing and testing self-assembling nanocomposites of metal oxides and graphene**—to greatly improve the capacity, power and cycle life of rechargeable lithium ion batteries for transportation and large-scale renewable energy storage.
- **Providing invited comprehensive reviews of the state of the science of energy storage technologies**—to explain the potential of major energy storage technologies for grid applications and, more importantly, to clearly identify advances necessary for widespread deployment.
- **Developing high-capacity redox flow chemistries**—to increase specific energy by as much as 70 percent and reduce system costs. New electrolyte additives and novel redox couples have been developed.



This artist's rendering of an upgraded vanadium redox battery shows how using both hydrochloric and sulfuric acids in the electrolyte significantly improves the battery's performance and could also improve the electric grid's reliability and help connect more wind turbines and solar panels to the grid.

WHY IT MATTERS

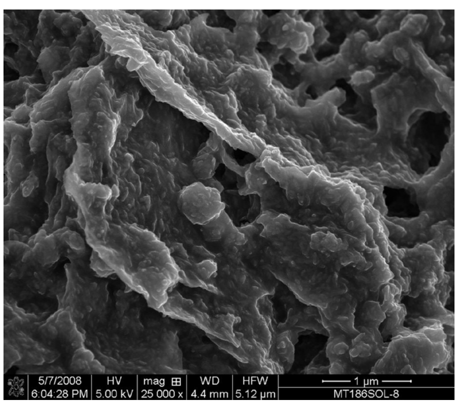
To deploy more energy-efficient vehicles and renewable energy sources, technologies are needed that can efficiently, safely and cost-effectively store energy. Although progress has been made in the last 20 years, significant improvements in the performance of batteries for renewable and transportation applications ultimately depend upon revolutionary breakthroughs in multifunctional nanomaterials, in materials considered for their performance and affordability and in the fundamental design of batteries. The work being done by our interdisciplinary teams of scientists is taking fundamental science through application to industrial partners.

FOCUS AREAS

Large-Scale Electrical Energy Storage to Improve Grid Reliability and Integrate Intermittent, Renewable Generation. The scientists are developing a deep understanding of the physical phenomena relevant to charge exchange and transport on the nanoscale and achieving cooperative phenomena in integrated complex structures on the macroscopic scale. For example, after using high-field nuclear magnetic resonance (NMR) spectroscopy to better understand cation hydration, additives were developed that increased the concentration of vanadium species in solution resulting in a 70% increase in specific energy while expanding the operational temperature range for the vanadium redox flow battery. Such advances are critical to achieve necessary life cycle costs and lifetimes for grid-related storage systems.

Nanostructured Materials for Advanced Energy Storage. Given that the performance of electrochemical storage devices ultimately depends on the properties of the electrode and electrolyte materials, emerging applications require revolutionary breakthroughs in the electrochemically active materials. Our team is gaining fundamental knowledge of the roles of nanostructures in electrochemical energy storage and desirable nanostructures for particular applications. For example, scientists published a study in *Science* that provides *in situ*, high-resolution transmission electron microscopy (TEM) images of electrode wires during real-time electrochemical cycling of a nanoscale battery. The study shows how the anode wires contort as a result of the huge volume expansion upon lithium insertion (charging). The work clearly identifies underlying chemical and microstructural transformations occurring during battery charge/discharge cycling and provides insights for building better batteries.

The team is also developing breakthrough materials and chemistries that may lead to higher energy and power densities, while not compromising battery life, safety, and cost. They are also developing computational models and *in situ* characterization tools to understand different phenomena in materials.



High-capacity, safe batteries are needed for efficient hybrid or electrical vehicles and for storing and releasing electricity from intermittent power sources. Scientists at Pacific Northwest National Laboratory and Princeton University, using EMSL resources, devised a method for building titania and SnO_2 functionalized graphene sheets (FGS) that significantly improve the performance of lithium ion batteries. This new titania/FGS composite has twice the capacity at high charge/discharge rates as batteries using conventional titania/carbon anodes.

WHAT'S NEXT

TMSI continues to advance the frontiers of materials science in energy storage with emphasis on technologies "beyond lithium ion." Storage systems such as lithium-sulfur and rechargeable lithium-air have potential to increase energy density beyond that of current Li-ion batteries. For grid-scale storage, cost reduction through improved materials and system design is the primary emphasis. Future work focuses on manufacturing electrodes and novel battery architectures in collaboration with industrial partners.

For example, we are working with Vorbeck Materials to scale up the manufacturing of nanocomposite electrodes for commercial applications. In addition, we are working with EaglePicher Technologies, LLC., on an Advanced Research Projects Agency for Energy grant to scale the novel planar sodium-beta battery architecture into a 5-kW battery for grid applications.

SPONSORS

Laboratory-Directed Research and Development, Department of Energy, and private industry

RESEARCH TEAM

The team for this work is led by Jun Liu and Gordon Graff. It includes a host of talented scientists, such as Yuliang Cao, Daiwon Choi, Jun Cui, Dan DuBois, Dehong Hu, Jian Zhi Hu, Jun-Jung Lee, John Lemmon, Yuehe Lin, Vijayakumar Murugesan, Zimin Nie, Juan Li, Xiaolin Li, Kevin Rosso, Laxmikant Saraf, Birgit Schwenzer, Yongsoon Shin, Vince Sprenkle, Maria Sushko, Chongmin Wang, Li-Qiong Wang, Wei Wang, Gordon Xia, Jie Xiao, Wu Xu, Z Gary Yang, Ji-Guang (Jason) Zhang, and Xiao-Dong Zhou of PNNL; Michael Pope and Ilhan Aksay of Princeton University; and many others.

SELECTED REFERENCES

Yang Z, J Zhang, M Kintner-Meyer, X Lu, D Choi, J Lemmon, and J Liu. 2011. "Electrochemical Energy Storage for Green Grid." *Chemical Reviews*, DOI 10.1021.

Huang JY, L Zhong, CM Wang, JP Sullivan, W Xu, LQ Zhang, SX Mao, NS Hudak, XH Liu, A Subramanian, HY Fan, L Qi, A Kushima, and J Li. 2010. "In Situ Observation of the Electrochemical Lithiation of a Single SnO_2 Nanowire Electrode." *Science* **330**(6010):1515-1520.

Li L, S Kim, W Wang, M Vijayakumar, Z Nie, B Chen, J Zhang, G Xia, J Hu, GL Graff, J Liu, and ZG Yang. 2011. "A Stable Vanadium Redox-Flow Battery with High Energy Density for Large-Scale Energy Storage." *Advanced Energy Materials*, DOI 10.1002 (11 Mar 2011).

Wang D, R Kou, D Choi, Z Yang, Z Nie, J Li, LV Saraf, D Hu, J Zhang, GL Graff, J Liu, MA Pope, and IA Aksay. 2010. "Ternary Self-Assembly of Ordered Metal Oxide-Graphene Nanocomposites for Electrochemical Energy Storage." *ACS Nano* **4**(3):1587-1595.

Lu X, G Xia, JP Lemmon, and Z Yang. 2010. "Review: Advanced Materials for Sodium-Beta Alumina Batteries: Status, Challenges and Perspectives." *Journal of Power Sources* **195**:2431-2442.

Choi D, D Wang, IT Bae, J Xiao, Z Nie, W Wang, VV Viswanathan, YJ Lee, JG Zhang, GL Graff, Z Yang, and J Liu. 2010. "$LiMnPO_4$ Nanoplate Grown via Solid-State Reaction in Molten Hydrocarbon for Li-Ion Battery Cathode." *Nano Letters* **10**(8):2799-2805.

ABOUT PNNL

PNNL is located in Richland, Wash., has approximately 4,700 staff, and $1.1 billion in business volume in fiscal year 2009. In the quest for knowledge discovery, PNNL marshals interdisciplinary research teams, collaborates with a range of partners, and leverages research funding to maximize results. Our staff, facilities, capabilities, and approach to inquiry and innovation have established PNNL as a premier science and technology enterprise.

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