Frontiers in
Energy Research

Newsletter

Summer 2017

Scientific Playgrounds Accelerating Clean Energy Research

Department of Energy provides extraordinary resources integral to many EFRC scientific breakthroughs

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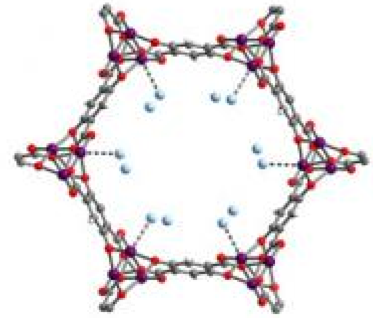
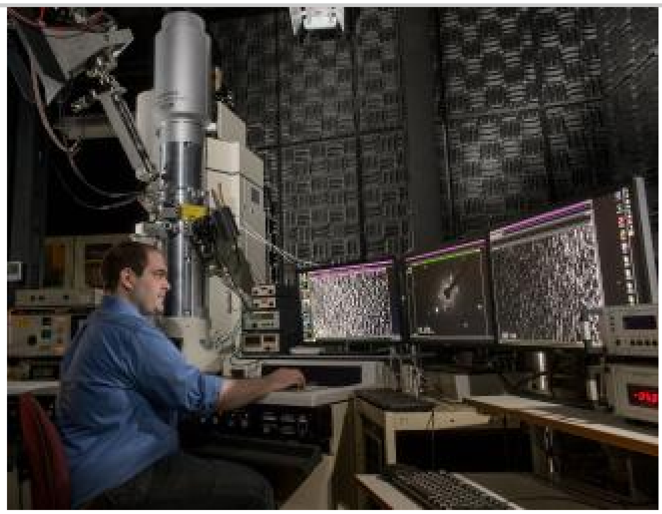
When taking on today's most exciting clean energy research, Energy Frontier Research Center (EFRC) scientists are bound to run into challenges requiring exotic instrumentation or uncommon techniques they do not have at their disposal. Luckily, for many such cases, the Department of Energy (DOE) has an answer: user facilities, the playgrounds of the scientific world, where researchers can access extraordinary resources to further their scientific goals. These user facilities and their state-of-the-art capabilities are invaluable for the EFRC mission.



(Left): Using this gas cell, CGS researchers observed gases adsorbing on MOF pore walls with in situ synchrotron X-ray diffraction. **(Right)**: Diffraction data showing argon atoms (blue) occupying multiple adsorption sites in the MOF Co_2(dobdc). *Modified images courtesy of the Royal Society of Chemistry and the associated scientists*

The DOE is home to 28 user facilities spanning many disciplines. Of those, 12 are in Basic Energy Sciences, which is also home to the EFRCs. Use of the facilities is awarded competitively and is free of charge for non-proprietary work, including research to be published in peer-reviewed journals. Generally, scientists apply for use of an instrument such as a synchrotron beamline or powerful microscope. If their experiments are approved, the scientists travel to the facility — often just for a few hours or days, but sometimes for many months — to conduct their experiments before returning home. Some EFRCs include user facility scientists as members, enabling frequent, high-level collaboration.



The Intermediate Voltage Electron Microscopy-Tandem Facility at Argonne National Laboratory was used by EDDE researchers to irradiate metal alloys with high-energy ions while monitoring the formation of defects. *Image courtesy of Argonne National Laboratory*

User facilities cover a broad scope of capabilities and are used by EFRC researchers for everything from nanoscience expertise to neutron scattering and supercomputing resources. Here are a few examples of EFRC breakthroughs made possible by user facilities.

Observing gas adsorption with synchrotron X-rays

High-flux, broadband X-rays are a coveted resource, and accelerating electrons in a synchrotron light source is the best-known way to make them. The Center for Gas Separations Relevant to Clean Energy Technologies (CGS) uses the Advanced Light Source (ALS), a user facility at Lawrence Berkeley National Laboratory, to directly observe how gas molecules adsorb in the pores of metal-organic frameworks (MOFs). Efficient gas separations, including the capture of carbon dioxide released when burning fossil fuels, could drastically reduce the carbon footprint of many industrial processes. MOFs, porous crystals that act like molecular sponges, make excellent adsorbents for many small molecules such as carbon dioxide and hydrogen. This makes them promising materials for gas separations, but the ways gases interact with MOF pore walls at various pressures are not fully understood.

Leveraging the remarkable flux of the ALS, CGS researchers have developed gas cells that allow them to collect single-crystal X-ray diffraction data from the MOFs at controlled gas pressures. The researchers dose the MOFs with gases and watch as the adsorbed species fit into unique adsorption sites within each pore. Gases adsorb to the strongest binding sites, and as the pressure increases, additional sites are filled. This fundamental understanding of an adsorption mechanism, realized thanks to the capabilities of both the CGS and the ALS, will guide future development of MOF materials for energy-efficient gas separations.

Understanding radiation damage in alloys

Safe nuclear power requires materials that can withstand high radiation doses at elevated temperature, which in turn necessitates knowing how materials respond to these extreme environments. When studying a promising class of radiation-resistant materials called concentrated solid-solution alloys, the Energy Dissipation to Defect Evolution (EDDE) EFRC has utilized many user facilities' advanced characterization capabilities. An EDDE team directly observed defect propagation under high radiation doses using the Intermediate Voltage Electron Microscopy (IVEM)-Tandem Facility at Argonne National Laboratory. This user facility allowed the team to bombard their samples with krypton ions inside an electron microscope, providing real-time insight into defect propagation and confirming hypotheses based on other experimental and molecular dynamics results.

Another team included neutron scattering from the Spallation Neutron Source in their characterization toolbox to understand how atoms in these metal mixes organize. Instead of finding total randomness, as expected, their results show short-range order throughout the materials due to preferential bonding between certain atoms. These findings will help the nuclear power community design better radiation-resistant materials.

Studying lithium-ion battery components

Improvements to lithium-ion battery chemistry promise to advance energy storage for devices from cell phones to electric cars. Researchers from the Nanostructures for Electrical Energy Storage (NEES) EFRC, including members of Sandia National Laboratories' Center for Integrated Nanotechnologies user facility, one of five DOE nanoscale science research centers, have developed new methods to probe the electrochemistry of nanoscale electrode materials. Through this collaboration, the NEES team developed a technique to measure electron diffraction patterns of nanoscale electrode materials as they react.

The electrode material, here titanium dioxide, accepts lithium ions as the battery is charged. As this happens, the team measures changes in individual crystal domains' structure using diffraction patterns collected with an electron microscope. With this new technique, they demonstrated that crystal domains smaller than around 25 nanometers react through a different mechanism than the bulk material, and their results suggest the smaller domains could lead to batteries with faster kinetics. Previous attempts to study this system were limited to measuring the average composition of many crystals. Because the new technique developed by NEES researchers isolates diffraction patterns from individual crystal domains, behaviors unique to nanoscale electrode materials were observed. The NEES team's exciting results offer the community new tools to understand electrode materials and pave the way for the better design of nanostructured battery components.

Today and tomorrow at user facilities

User facilities provide EFRCs with the tools needed to make the rich scientific discoveries discussed here. Due to their ever-advancing capabilities, these facilities allow researchers to understand energy-relevant systems with precise temporal and spatial resolution. Moving forward, these resources will be critical in pushing the boundaries of clean energy science and developing the disruptive energy technologies our society needs.

Acknowledgments

CGS: Gonzalez et al., 2017, were supported through the Center for Gas Separations Relevant to Clean Energy Technologies (CGS), an Energy Frontier Research Center (EFRC) funded by the Department of Energy (DOE), Office of Science, Basic Energy Sciences. This research used resources of the Advanced Light Source and the Molecular Foundry, which are supported by the Director, DOE Office of Science, Basic Energy Sciences.

EDDE: Lu et al., 2016, were supported as part of Energy Dissipation to Defect Evolution (EDDE), an EFRC funded by the DOE, Office of Science, Basic Energy Sciences. Ion beam work was performed at the University of Tennessee/Oak Ridge National Laboratory (ORNL) Ion Beam Materials Laboratory located on the campus of the University of Tennessee, Knoxville. The molecular dynamics simulation was performed using the supercomputer of Flux at University of Michigan. Cross-sectional transmission electron microscopy (TEM) was conducted in the Michigan Center for Material Characterization of the University of Michigan. In situ TEM during ion irradiation was carried out using the IVEM-Tandem Facility at Argonne National Laboratory.

Zhang et al., 2017, were supported as part of EDDE, an EFRC funded by the DOE, Office of Science, Basic Energy Sciences. Neutron diffraction measurements used resources at the Spallation Neutron Source, a DOE Office of Science user facility operated by ORNL. The X-ray pair distribution function and extended X-ray absorption fine structure measurements were conducted at the Cornell High Energy Synchrotron Source (CHESS), which is supported by the National Science Foundation and the National Institutes of Health/National Institute of General Medical Sciences.

NEES: Zhong et al., 2017, were supported by National Science Foundation through University of Pittsburgh (S.X.M.) and the Nanostructures for Electrical Energy Storage (NEES), an EFRC funded by the Department of Energy, Office of Science, Basic Energy Sciences. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science user facility operated for DOE's Office of Science. Sandia National Laboratories is a multiprogram laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for DOE's National Nuclear Security Administration.

More Information

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Stephen Meckler is a graduate student in the chemistry department at the University of California, Berkeley. He is a member of the Center for Gas Separations Relevant to Clean Energy Technologies (CGS) Energy Frontier Research Center. His research focuses on developing and studying porous materials for gas separation membranes, including porous polymers, metal-organic frameworks and composites thereof.

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