DISCOVERY

Science Frontiers 2013



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Pacific Northwest National Laboratory (PNNL), a U.S. Department of Energy Office of Science Laboratory, is pushing the frontiers of science in areas that are critical to the nation's security, health and prosperity.

PNNL's science and technology base ranges from basic research in chemistry, biology and physics, to applied sciences and technology development addressing some of the nation's most pressing challenges in energy, environment and national security.

This brochure highlights a few examples of PNNL's research at the frontiers of science and technology—research that is pushing the boundaries of knowledge and improving lives every day.



Environmental Molecular Sciences Laboratory (EMSL)

EMSL is a national scientific user facility, a federally funded community resource located at PNNL. EMSL uses a peer-review process to grant access to scientists from universities, industry and government agencies who seek out its unique ability to integrate state-of-the-art facilities, world-class expertise and advanced scientific instruments for their most challenging research.

EMSL offers more than 150 cutting-edge instruments, many of them one-of-a-kind tools. Over 10,000 scientists supported by agencies such as the Department of Energy, National Institutes of Health, Environmental Protection Agency and the Department of Defense have conducted research at EMSL.

Working with General Motors, EMSL researchers have boosted the storage capacity and reliability of lithium ion batteries; these advances will yield longer-lasting, cheaper rechargeable batteries and will make electric vehicles more competitive with conventional ones.

Chemical Conversion: Key to Sustainable Energy

PNNL is a world-renowned center for research in catalysis: the control of chemical reactions. At PNNL's Institute for Integrated Catalysis, teams are unlocking the basic workings of numerous catalysts to create abundant low-cost fuel from domestic feedstocks.

At the Center for Molecular Electrocatalysis, PNNL scientists created a catalyst that can produce 100,000 hydrogen molecules per second, spurring the commercial viability of fuel from domestic feedstocks.

Over the next five years, PNNL scientists aim to decrease the cost of biomass conversion to fuel by 50% and achieve ultra-low-temperature exhaust emission control for high-efficiency engines, increasing vehicle fuel economy by 50%.

PNNL teams are also developing new approaches to electrical and chemical energy conversion that will be applied in low-temperature fuel cells to avoid the use of expensive, scarce precious metals and potentially use carbon dioxide as a fuel feedstock.

Designing the Computing Systems of the Future and Tackling *Big Data*

PNNL is a world leader in computer performance and programming models and analysis, and in graph analytics—capabilities that help tackle challenges in science that require extreme scale computing. Scientists at PNNL build methodologies to model next-generation computer architectures that will consume less power, be more resilient and allow real-time computing to understand the operations of the electric grid.

Recently, PNNL established the Northwest Institute of Advanced Computing, a joint venture between the University of Washington and PNNL where researchers will tackle "big data" for challenges ranging from climate change to energy management.

PNNL also set up the **Collaboratory on Mathematics** for Mesoscopic Modeling of Materials to support fundamental scientists with a new way of describing particle/matter interactions at a very small scale. The goal is to enable design of new materials and properties that will be customized according to the needs of the problem—a capability currently unavailable at the different scales needed by the scientists.

Molecular-Scale Imaging

Scientists at PNNL are developing a unique set of instruments allowing researchers to move from mere observation of model systems to studying, manipulating and controlling complex biological, environmental and energy systems at the molecular scale. These imaging tools will accelerate discoveries that impact society's energy, environmental and health needs.

PNNL will develop expertise and capabilities for the next generation of structural biology with whole cell function correlation, the discovery of new energy conversion and storage materials, and the analysis of environmental particles such as aerosols for reducing uncertainties in climate modeling and understanding the impacts of these particles on human health.





Understanding Climate Change

PNNL scientists are international leaders in understanding the dynamics of the integrated Earth system—atmosphere, surface and subsurface—and its interactions with energy, land use and other human systems. This leadership includes providing technical direction and oversight for the Atmospheric Radiation Measurement (ARM) Climate Research Facility, a unique observational resource. In addition, PNNL scientists connect these and other measurements with integrated, state-of-the-art models of regional and global changes.

And at the Joint Global Change Research Institute, a collaboration between PNNL and the University of Maryland, researchers apply expertise in economic and policy analysis to assess climate change impacts, and mitigation and adaptation options for policy makers.

Predicting Biological System Behavior

Micron-size microorganisms can do amazing things such as produce biofuels from waste products or sunlight. Scientists at PNNL are analyzing microorganisms and their communities in the laboratory and field to predict, or simulate, their response under specific environmental conditions. Research is yielding insights that scientists are applying to the nation's energy, environmental and health challenges. Examples include sustainable hydrogen production by photosynthetic bacteria, and modeling how subsurface contamination can move or stay in place.

Microbial community research at PNNL focuses on environmental and energy processes and development of new biological processes. The health-related research builds on PNNL's unique ability to measure life's building blocks—proteins and metabolites—and identify molecular signatures to detect disease early and predict response to drugs and environmental exposures. PNNL's Center for Systems **Biology of Enteric Pathogens** applies expertise in microbial systems to human health, and the Proteomics Research Resource provides cuttingedge measurements of proteins and metabolites to solve compelling biological problems.



Understanding Mesoscale Science to Design New Materials for Sustainable Energy

Mesoscale science is not about length or time; it is about the vital complexity that occurs between or in the middle of smaller and larger scales. This complexity gives rise to new, unexpected phenomena that could aid in creating materials for long-lasting batteries or turning carbon dioxide into fuel. At PNNL, we build upon our knowledge of how molecular and nanoscale systems behave to learn new fundamental principles about phenomena that emerge from the interactions of these simpler systems in more complex assemblies. We make these discoveries with new experimental and computational tools that we devise. Our foundational work is important for the development of catalytic processes for energy, novel energy storage and magnetic materials, new generations of sensors and membranes to control transport and separations processes.

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Biological Sciences Facility

BSF houses state-of-the-art analytical equipment and powerful computing capabilities that enable scientists to address challenges in energy, national security and human health.

Computational Sciences Facility CSF has 12,500 square feet of energyefficient raised floor space supporting computing for national mission areas. It is home to Olympus and the Center for Adaptive Supercomputing Software.

Physical Sciences Laboratory

PSL is home to the Institute of Integrated Catalysis and the Center for Molecular Electrocatalysis and also houses PNNL's site for the Joint Center for Energy Storage Research.

Atmospheric Measurements Laboratory

Leading research facility for understanding the aerosol particle lifecycle and associated effects on climate using unique instrumentation and atmospheric chambers.

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EMSL

EMSL, a national scientific user facility at Pacific Northwest National Laboratory, provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of DOE and the nation.

Offsite Facilities

Joint Global Change Research Institute

A Pacific Northwest National Laboratory and University of Maryland partnership, located in College Park, Md., where research centers on understanding the interactions between climate, energy, economic activity and the environment.

The Northwest Institute for Advanced Computing

A joint partnership between the University of Washington located in Seattle, Wash., and Pacific Northwest National Laboratory in Richland, Wash. Researchers from both institutions will focus on ensuring that the next generation of computers and methods used to run them can address the challenges ranging from climate change to energy management.

FY12 PNNL Facts & Figures

- » One of the DOE's 17 national laboratories where interdisciplinary teams advance science and technology and deliver solutions to America's most intractable problems.
- » Among top 1% of research institutions in publications and citations in a variety of disciplines.
 - **\$1.0B** Operating Budget 4,454 Scientists, Engineers and Staff **1,041** Peer-Reviewed Publications **176** Invention Disclosures **44** Patents Granted 3 R&D 100 and FLC Awards

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