Powering Innovation with Fundamental Science

How PNNL accelerates foundational research in climate, energy, biology, and computing

Pacific Northwest NATIONAL LABORATORY

Fundamental research is critical for maintaining U.S. economic prosperity and supporting national priorities in climate, clean energy, pandemic resilience, and innovation. PNNL integrates basic energy sciences, advanced scientific computational research, and biological and environmental research to accelerate discoveries in energy storage, human health, environmental stewardship, cybersecurity, quantum information sciences, and other key fields.

PREDICTING CLIMATE CHANGE AND ITS IMPACTS

PNNL is internationally recognized for climate and Earth system science research, particularly in atmospheric science, hydrology, biogeochemistry, and integrated human-Earth system modeling. For example, PNNL scientists are using data collected by the *Atmospheric Radiation Measurement (ARM) User Facility* and analyzed by the *Environmental Molecular Science Laboratory (EMSL)* to improve understanding of how atmospheric aerosol particles interact with clouds to influence the global radiation budget and extreme precipitation events.

Another area of focus is coastal regions, which are increasingly vulnerable to sea level rise, stronger storms, and other environmental changes. Information from these and many other research activities is used to develop increasingly sophisticated models to simulate future Earth system changes, which is critical for informing local, state, regional, national, and international actions to mitigate and adapt to climate change in ways that promote sustainable economic growth, environmental justice, and other important goals.

CLEANER ENERGY THROUGH CHEMICAL AND MATERIALS SCIENCE

The transition from fossil fuels to cleaner energy systems is one of the grand challenges of the 21st century. Major improvements in chemical and materials transformations will be critical to achieving the goal of decarbonizing the nation's energy system by 2050. PNNL researchers are making critical advances in materials for next-generation batteries, catalysts that turn waste into fuel, and other game-changing technologies. Two new DOE facilities at PNNL—the *Energy Sciences Center (ESC)*, funded by the Office of Science, and the *Grid Storage Launchpad (GSL)*, funded by the Office of Electricity—will provide leading-edge capabilities to advance and accelerate catalyst and battery design.

PNNL is also exploring emerging opportunities in atomically precise synthesis for advanced materials development and applications, including world-leading expertise in the science of synthesis. Novel technical approaches will yield breakthroughs for next-generation microelectronics, energy-efficient materials, and quantum information sciences.

BUILDING THE BIOECONOMY

Advances in biotechnologies such as gene editing and DNA synthesis—coupled with the physical sciences, engineering, and computer science—have led to the rapid transformation of biology into a more quantitative and agile discipline with an emerging capability to rationally design synthetic biological components, organisms, and systems. Unfortunately, biological systems also present risks; the COVID-19 pandemic has starkly illustrated the importance of addressing natural threats posed by traditional and emerging bioagents.

PNNL's fundamental bioscience program is focused on predictive phenomics, which is understanding, predicting, and controlling how a biological system responds to changes in its genome and/or its environment. EMSL capabilities are instrumental in interrogating and interpreting the functions of biological systems at the scope and scale needed to develop predictive understanding. The ultimate goal is the rational design of biological systems for applications spanning the bioeconomy—from the bio-based production of materials, chemicals, and fuels to improved strategies for countering biological threats, and to the design of hardier, more nutritious crops.

ACCELERATING SCIENCE WITH CUTTING-EDGE COMPUTING

PNNL is a recognized leader in data science and machine learning for scientific discovery, and these approaches have underpinned recent advances across a range of disciplines. For example, PNNL scientists are using and interpreting deep neural networks in physical chemistry, modeling interactions among water molecules, and finding information about how these molecules arrange and cluster at the most fundamental level. PNNL's approach to machine reasoning also underpins our work in autonomic resilience in cybersecurity, leading to control systems capable of proactively identifying and responding to threats.

PNNL researchers are developing applications for DOE's Exascale Computing Project, partnering with industry on next-generation architectures, and participating in three quantum computing centers. This work includes the creation of design concepts for new heterogeneous systems-on-a-chip that converge data, simulations, artificial intelligence, and data analytics. The development of new quantum algorithms and simulations will also accelerate studies of complex, correlated chemical systems at unprecedented levels of accuracy. The combination of high-performance computing, using platforms such as the PNNL-developed NWChem software, with future quantum computers will enable the rapid discovery of new materials and catalysts, thereby accelerating the transformation of our energy systems.

ABOUT PNNL

Pacific Northwest National Laboratory advances the frontiers of knowledge, taking on some of the world's greatest science and technology challenges. Distinctive strengths in chemistry, Earth sciences, biology, and data science are central to our scientific discovery mission. PNNL's research lays a foundation for innovations that advance sustainable energy through decarbonization and energy storage and enhance national security through nuclear materials and threat analyses.

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