Pacific Northwest
NATIONAL LABORATORY

Proudly Operated by **Battelle** *Since 1965*

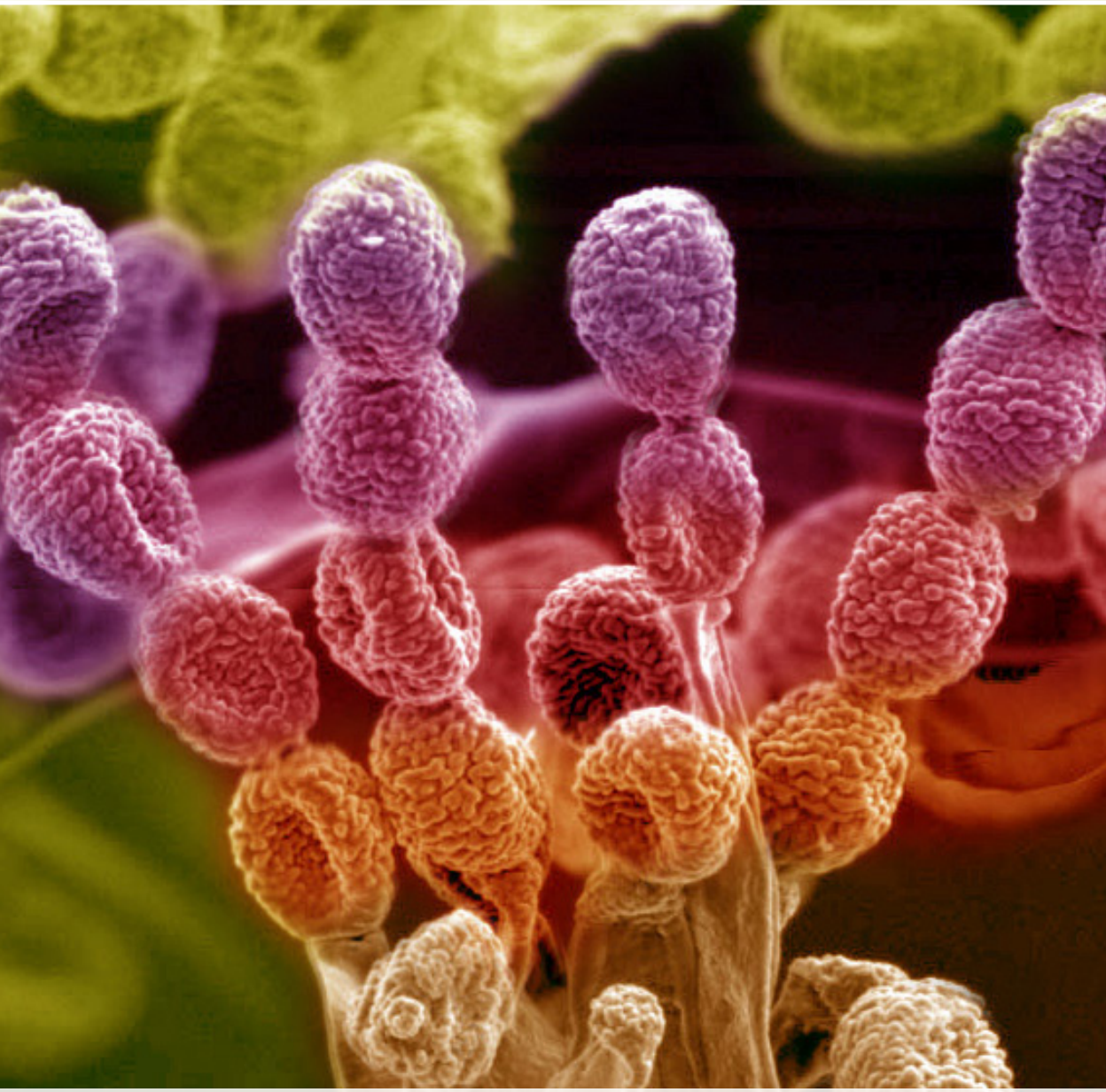
Science Frontiers 2014

Pacific Northwest National Laboratory (PNNL) is a U.S. Department of Energy (DOE), Office of Science Laboratory, operated by Battelle. PNNL is changing the world by addressing the most important questions on the frontiers of science, advancing understanding of nature and the planet, and providing the scientific foundations for technological innovation.

With substantial science and technology capabilities in many disciplines, including biology, chemistry, physics, computational sciences, and materials science, PNNL's research spans fundamental and applied sciences to technology development and commercialization efforts and leverages partnerships with other national laboratories, universities, and private firms.

This brochure highlights PNNL's research at the frontiers of science and technology—research on the leading edge, pushing the boundaries of knowledge and improving lives every day.

About the cover: A new transcriptomics-based model accurately predicts how much isoprene the bacterium *Bacillus subtilis* produces and is an early result in generating renewable fuels using bacteria. Support for this work was provided by DOE's Office of Biological and Environmental Research through the PNNL Foundational Scientific Focus Area, as well as Washington State University and the Washington State STAR researcher program. This work is part of a research campaign at PNNL's Environmental Molecular Sciences Laboratory: *Making Isoprene from Biomass Material Using Bacillus Species.*



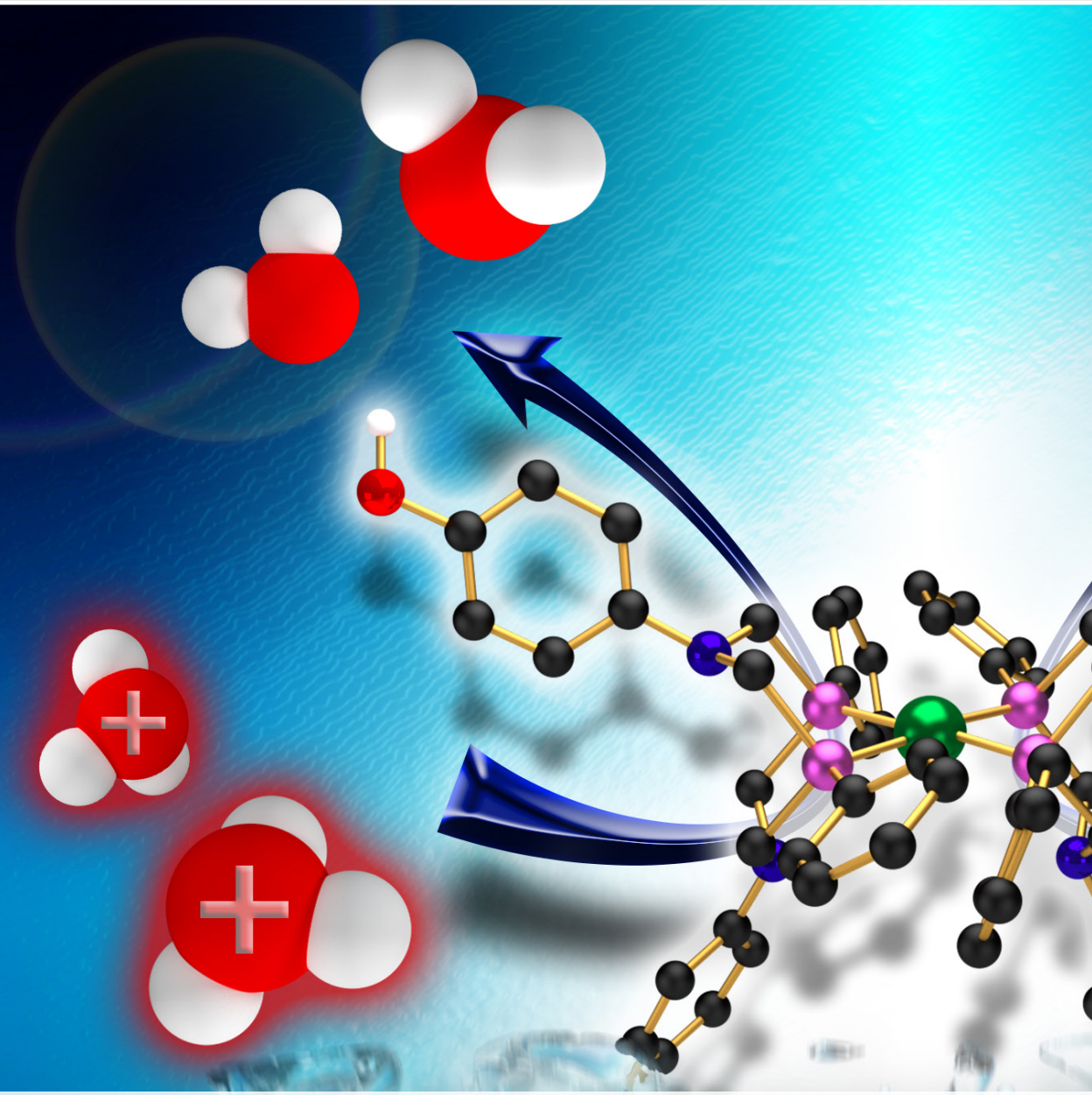
Predicting Behavior in Biological Systems

In recent decades, scientists have made substantial progress in understanding individual microorganisms. However, understanding the behavior of microorganisms in their communities is a frontier that could unlock tremendous innovation potential, leading to breakthroughs in the production of inexpensive biofuels from wastes or sunlight and development of higher capacity, lighter, rechargeable batteries.

At PNNL, scientists are analyzing microorganisms and their communities in both the laboratory and the field to predict and simulate their behavioral responses to their environment. This research is yielding insights that are being applied to the nation's energy, environmental, and health challenges. PNNL's ongoing systems biology research includes efforts to produce hydrogen fuels using photosynthetic bacteria and to understand the role of microorganisms in climate change and its impacts.

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. As a leading climate research institution, PNNL also provides technical direction and oversight of the Atmospheric Radiation Measurement (ARM) Climate Research Facility, a unique array of observatories around the world that gather data on Earth's atmosphere, making it available to the scientific community. PNNL scientists integrate ARM observations with the Laboratory's advanced scientific instrumentation and high-performance computing resources to build advanced computer models that can be used to study climate from molecular to Earth system scales. 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.



Catalyzing Chemical Conversions: Key to Sustainable, Secure Energy

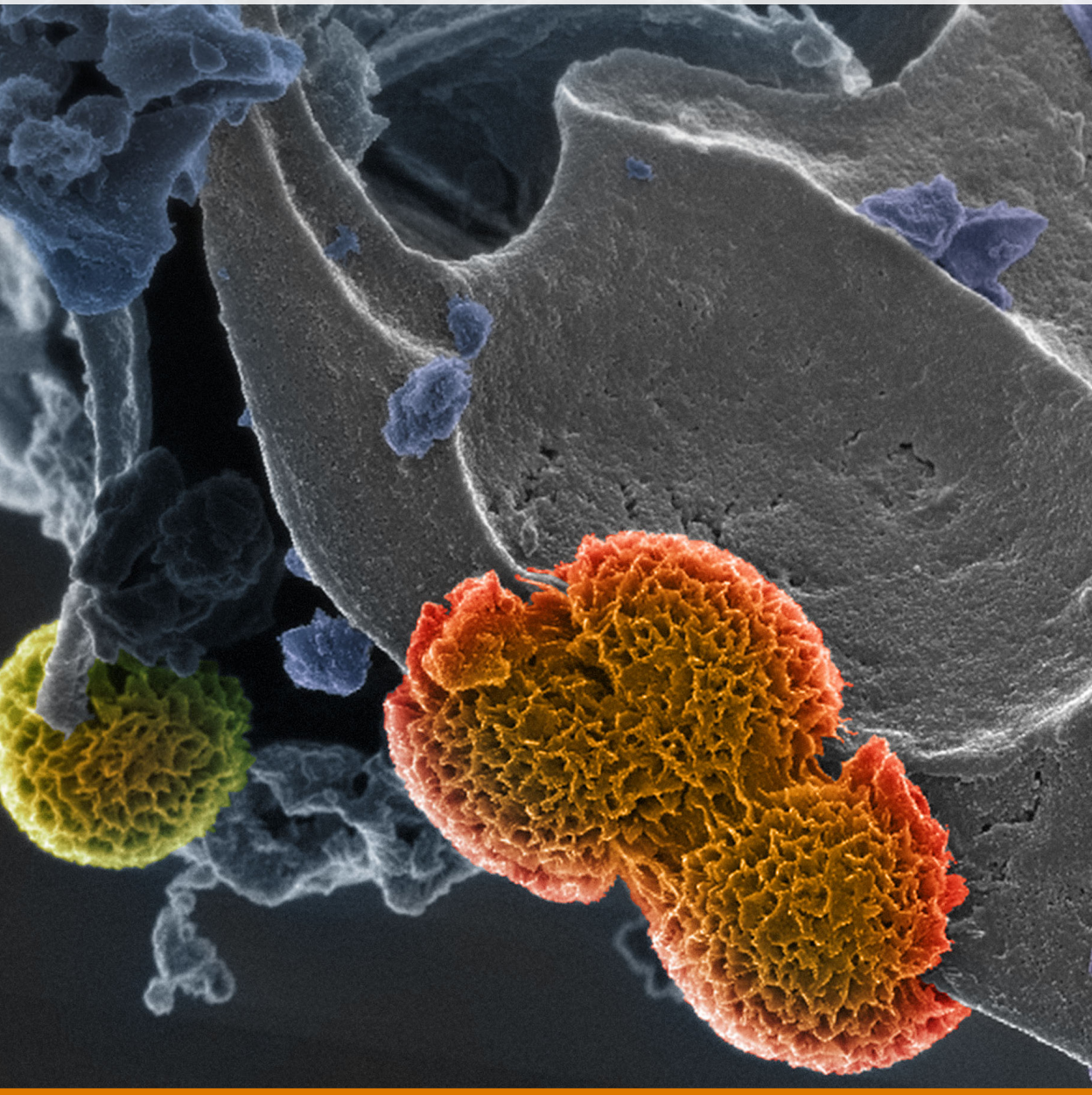
PNNL is a world-renowned center for research in catalysis—the control of chemical reactions. At PNNL's Institute for Integrated Catalysis, teams are unlocking the basic workings of numerous catalysts to create abundant, low-cost fuel from domestic feedstocks.

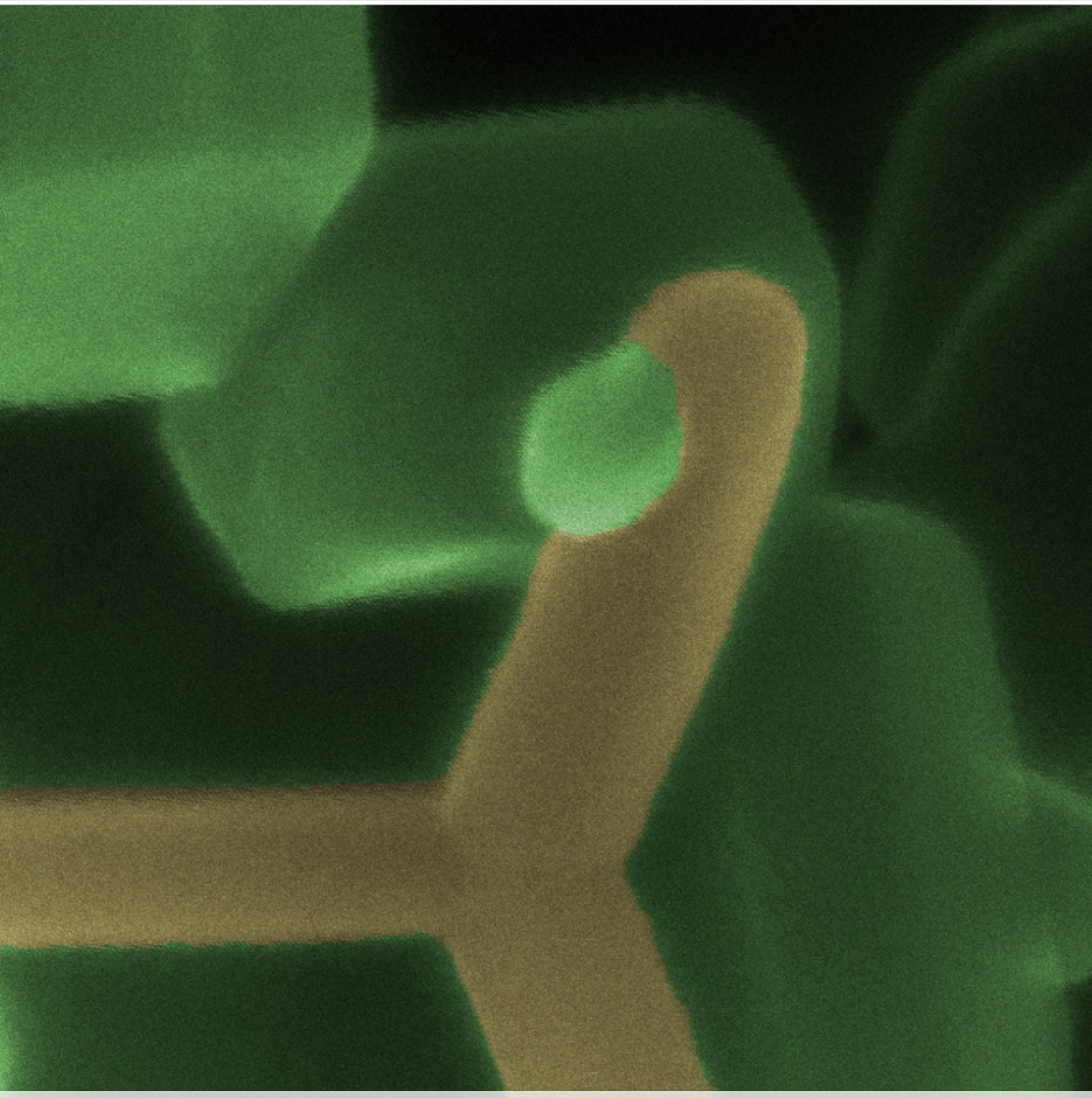
At the Center for Molecular Electrocatalysis, a DOE Energy Frontier Research Center at PNNL, scientists are using physical models to specifically design electrocatalysts that use iron and other earth-abundant metals to convert electrical energy into chemical bonds in fuels or, conversely, chemical energy into electrical energy. These catalysts will be essential in addressing worldwide problems of increasing energy demands, gradually depleting fossil fuel reserves, and increasing levels of atmospheric carbon dioxide.

Observing the World at the Smallest Scale: Molecular-scale Imaging

Unique instruments at PNNL allow researchers to move from laboratory observation of phenomena using models to direct, real-time observations of natural biological, environmental, and energy systems at the molecular scale. Imaging tools that equip scientists to study, manipulate, and control complex biological phenomena and chemical processes will accelerate discoveries that make energy cleaner and more affordable, improve human health, and spur the development of advanced materials.

Discovery science at PNNL employs a range of techniques and tools, including electron microscopes, mass spectrometers, scanning probe microscopes, high-resolution vibrational spectrometers, nuclear magnetic resonance, and atom probe tomography, to advance understanding of molecular-scale chemical and biological mechanisms.





Understanding Mesoscale

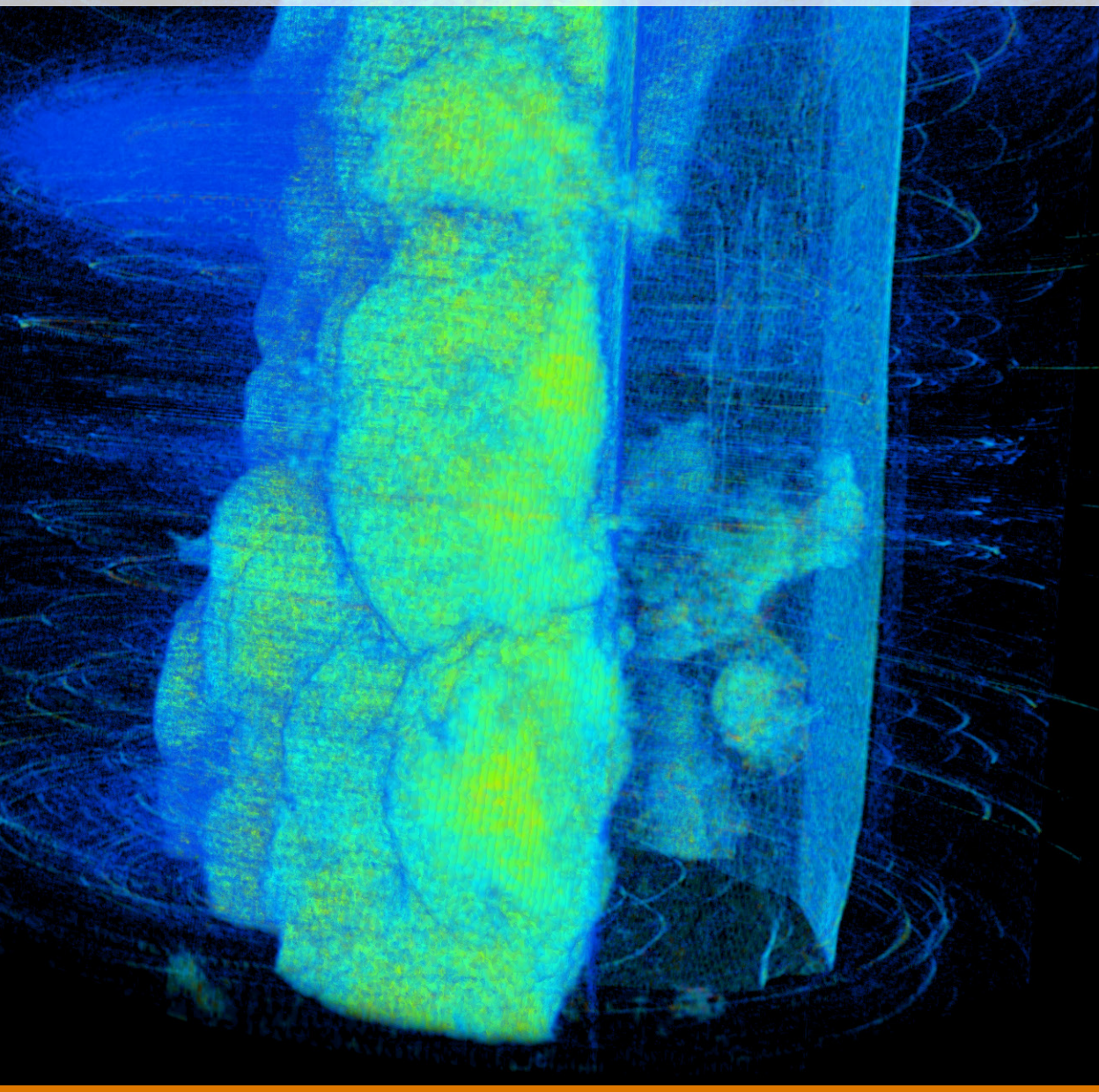
Mesoscale science involves the vital interactions that occur between the smallest (i.e., molecular) and larger scales. By observing and better understanding the complexities of mesoscale interactions, PNNL scientists are uncovering new, unexpected phenomena that could aid in creating a range of new materials to turn carbon dioxide into fuel, produce advanced batteries, and spur development of new medical devices and consumer products. At PNNL, scientists employ experimental and computational tools to understand molecular and nanoscale system behavior and uncover fundamental principles governing the interactions of these simpler systems as they form more complex assemblies. This foundational work is important for the development of catalytic processes for energy production, novel energy storage and magnetic materials, and new-generation sensors and membranes that control transport and separations processes.

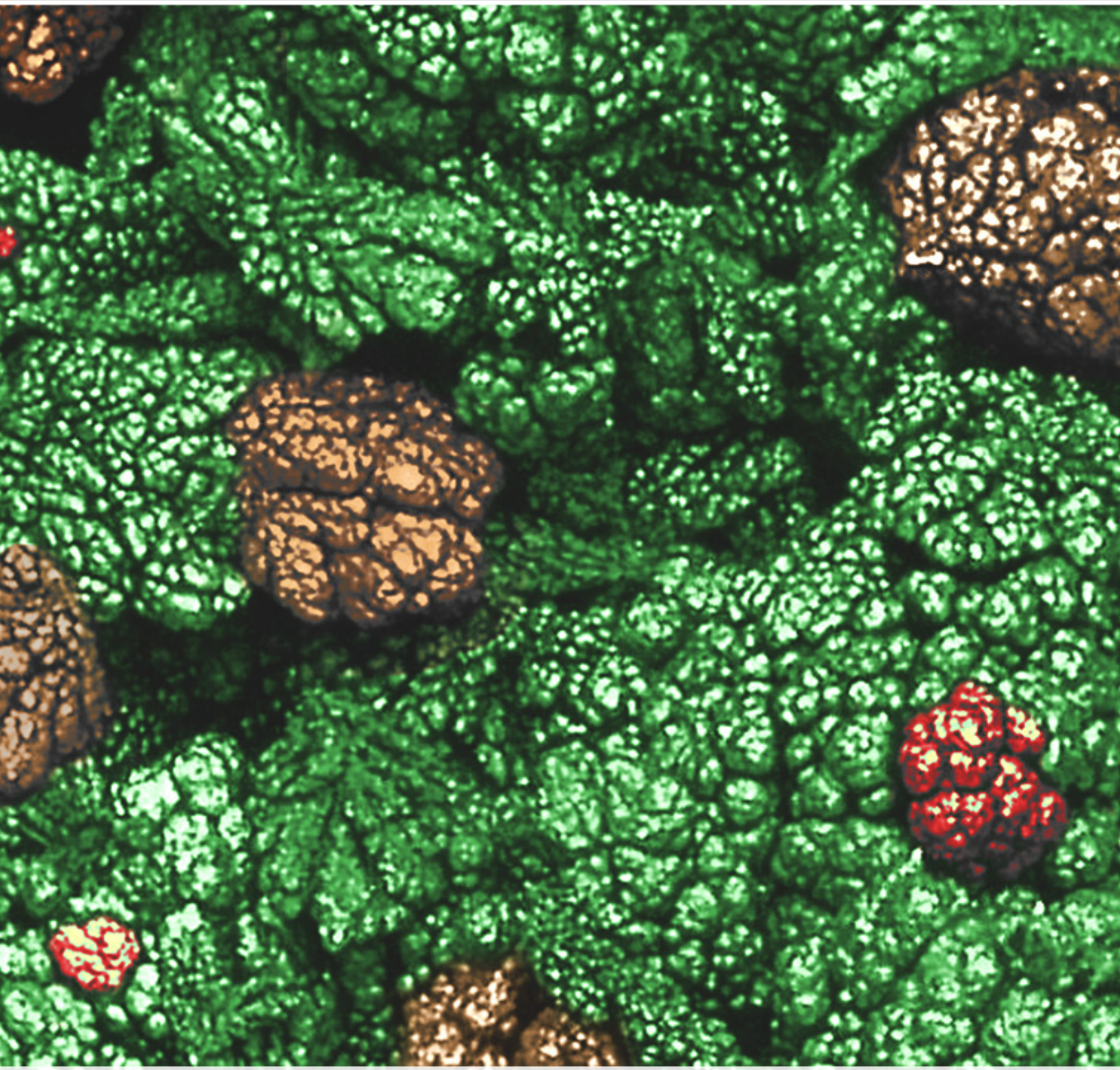
Advancing the Current State of Computing and Mathematics

PNNL is at the forefront of advanced computing systems and applications, improving performance, power, and reliability characteristics to maximize scientific discovery. These efforts affect a multitude of applications.

Founded jointly by PNNL and the University of Washington in 2013, the Northwest Institute for Advanced Computing, or NIAC, will unite research partners from diverse organizations and industry throughout the world to advance the use of computing in discovery affecting areas such as cybersecurity, healthcare, and urban science.

With the Collaboratory on Mathematics for Mesoscopic Modeling of Materials, PNNL is building mathematical foundations for understanding and controlling fundamental mechanisms at the mesoscale, the area between the size of a molecule and a cell, to enable breakthroughs in designing new and customizable materials used in electronics, medicine, and energy production and storage.





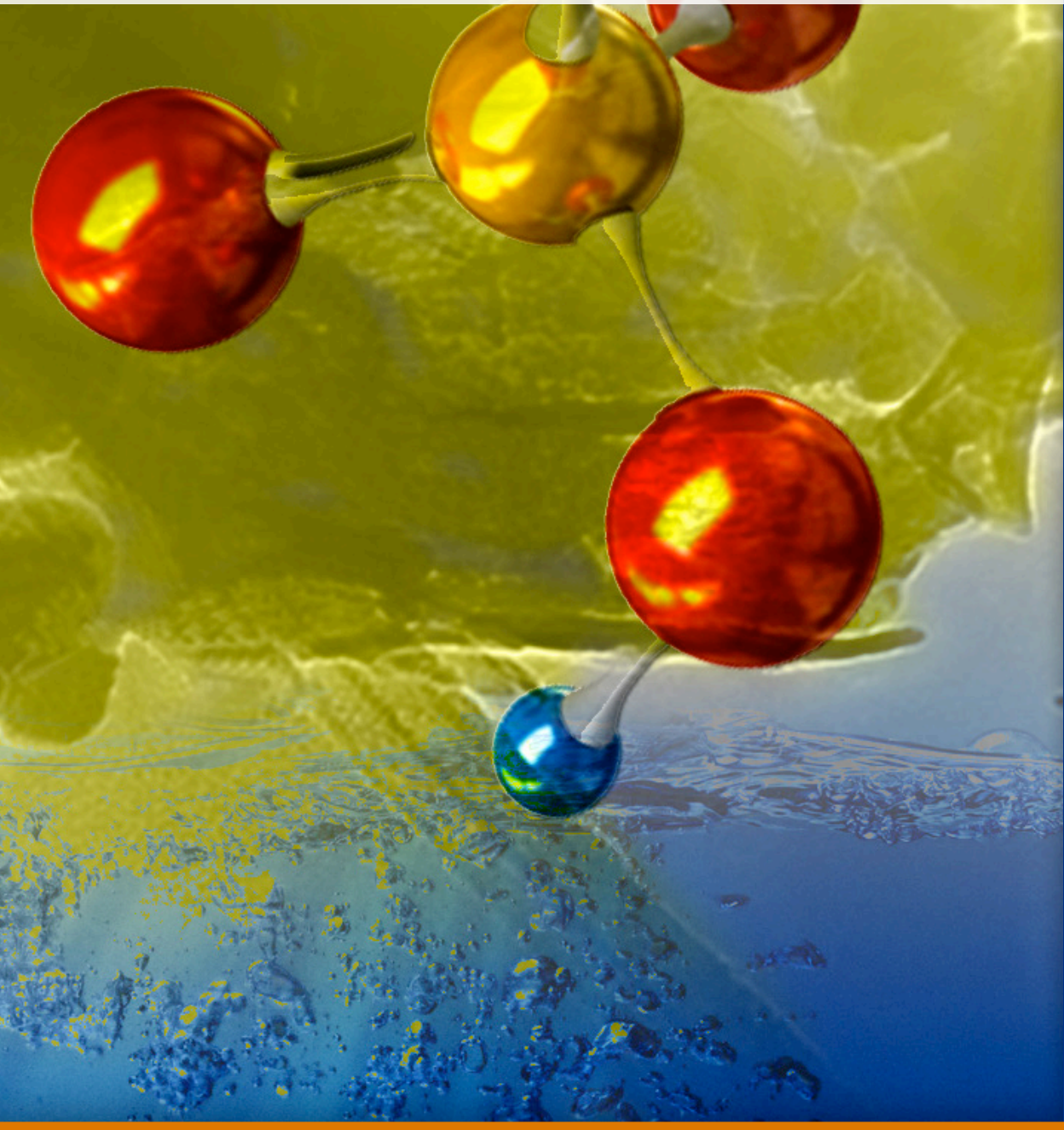
Ultra-Sensitive Nuclear Measurements: Bringing Dark Matter and Other Particles to Light

PNNL scientists are leading efforts to understand the dynamics of subatomic particles to see beyond the Standard Model of particle physics by seeking to bring elusive dark matter particles into the light. Dark matter, which may constitute as much as 80 percent of the universe, remains undetectable using conventional telescopic technologies. PNNL scientists are working to find the universe's "missing" mass to provide the first subatomic particle discovery beyond the Standard Model.

PNNL also is a contributor to the Majorana Demonstrator project, examining a never-before-observed radioactive decay, and plays a leading role in international experimental particle physics research through the Belle II project. PNNL's high-energy physics capabilities have grown out of its historic work to remove trace radioactivity from materials needed to build detectors for U.S. nuclear nonproliferation and treaty verification efforts.

Serving Science and the Scientific Community: The Environmental Molecular Sciences Laboratory (EMSL)

EMSL is a national scientific user facility—a federally funded laboratory operated by PNNL that serves as a resource to the science community at large. EMSL scientists work with researchers from universities, firms, and other laboratories around the country to address major science challenges, from efforts to understand the roles of clouds and aerosols in Earth's climate, engineer microbes for biofuels production and environmental cleanup, and comprehend the complex relationships between subsurface and terrestrial ecosystems. EMSL also is unique in its ability to integrate top scientific talent, leading-edge instruments, and high-performance computers to push the boundaries of science frontiers.



Facilities

Atmospheric Measurements Laboratory
AML is a leading research facility for understanding the aerosol particle life cycle and its associated effects on climate using unique instrumentation and atmospheric chambers.

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 energy-efficient raised floor space, supporting computing for national mission areas. It is home to PNNL Institutional Computing, the Center for Adaptive Supercomputing Software, and the Performance and Architecture Laboratory.

Environmental Molecular Sciences Laboratory
A national scientific user facility sponsored by the Department of Energy's Office of Biological and Environmental Research and located at PNNL, EMSL provides researchers access to integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences.

Joint Global Change Research Institute
Located in College Park, Maryland, JGCRI, a PNNL and University of Maryland partnership, centers its research on understanding the interactions between climate, energy, economic activity, and the environment.

Northwest Institute for Advanced Computing
Founded jointly by PNNL and the University of Washington in 2013, NIAC is both a physical and "virtual" collaborative center designed to maximize the impact of computing on transformative discoveries that fuel scientific and societal progress.

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.

PNNL Shallow Underground Laboratory
PNNL SUL is home to some of the world's most sensitive systems for radiation detection. The underground location provides shielding from cosmic-ray backgrounds, reducing them significantly from the earth's surface. SUL provides cleanroom space for the development of new materials and methods for environmental science, national security, and fundamental physics research.

PNNL: 2013 Facts & Figures

- More than 4,300 scientists, engineers, and staff
- Since 1965, 2,235 U.S. and foreign patents granted (36 U.S./49 foreign in 2013)
- Four Federal Laboratory Consortium and R&D 100 awards in 2013
- 1,168 peer-reviewed, published articles in 2013
- In 2013, PNNL ranked among the top 1 percent of research institutions in publications and citations in:
  - Biology and Biochemistry
  - Clinical Medicine
  - Environment and Ecology
  - Materials Science
  - Molecular Biology and Genetics
  - Chemistry
  - Engineering
  - Geosciences
  - Microbiology
  - Physics

For more information, contact:

Douglas Ray, Ph.D., Associate Laboratory Director
Fundamental & Computational Sciences Directorate
(509) 375-2500

Allison Campbell, Ph.D., Associate Laboratory Director
Environmental Molecular Sciences Laboratory
(509) 371-6000

Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle *Since 1965*

U.S. DEPARTMENT OF ENERGY

March 2014

PNNL-SA-101217