Pacific Northwest
NATIONAL
LABORATORY

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"Visualizing molecular structures and chemical composition in time and space–as events unfold–could revolutionize many areas of scientific inquiry."

Visualizing Chemistry, National Academy of Sciences, 2006

U.S. DEPARTMENT OF ENERGY

Chemical Imaging Initiative

Delivering New Capabilities for *In Situ*, Molecular-Scale Imaging

A complete, precise and realistic view of chemical, materials and biochemical processes and an understanding of the reactions occurring at the molecular level is vital to solving the nation's energy, environmental and security issues and to accelerating scientific progress. Numerous government-sponsored reports have identified imaging as critical for scientific advancement. However, current scientific instruments fail to reach the needed level of clarity. Instead, scientists must infer what is occurring from secondary sources and mathematical models.

At Pacific Northwest National Laboratory, the Chemical Imaging Initiative is developing a suite of tools with nanometer-scale resolution and element specificity. This instrumentation suite will allow scientists to go from observing to manipulating systems on a molecular level. These real-time, in situ tools will be achieved through three thrust areas:

Light-Source-Based Imaging

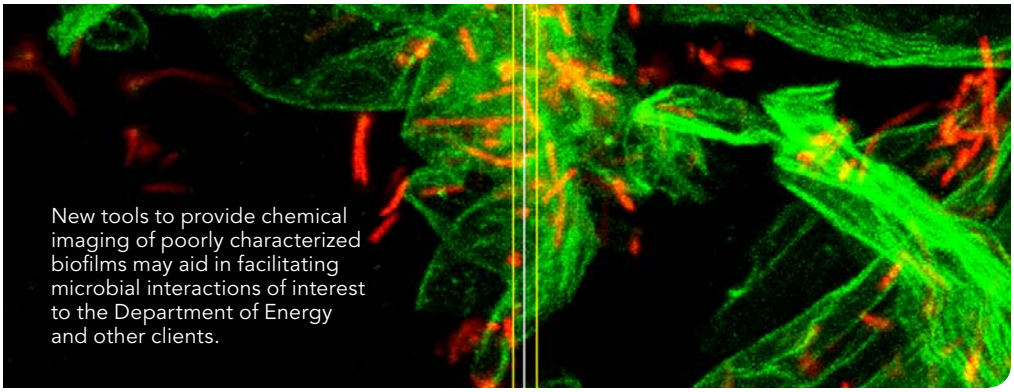
Develop probes for three-dimensional tomographic, structural and element-specific interrogation at the molecular level. The initiative is coupling light-source-based x-ray and vacuum ultraviolet probes with laboratory-based imaging capabilities. Use of these new techniques, for example, could provide an atomic-resolution, in situ "movie" of a functioning photocatalyst or clear characterizations of nanoporous materials and their active sites for batteries and biomolecules.

In-House Imaging

Combine microscopies to understand chemical and biological mechanisms. The initiative is coupling in situ electron microscopes, mass spectrometers, scanning probe microscopes, high-resolution vibrational spectrometers and atom probe tomography together or with light-source capabilities to image materials of importance to the nation's energy and environmental issues.

Multimodal Analysis and Integration Framework for Chemical Imaging

Integrate hardware and software for image reconstruction and feature extraction. The initiative is developing a flexible framework to facilitate analysis and integration across chemical imaging technologies. The framework will enable scientists to contribute their own tools. Tools and techniques for feature detection and distributed analysis and integration across different imaging technologies are being created, which could harness the computational power to solve fundamental scientific questions.



New tools to provide chemical imaging of poorly characterized biofilms may aid in facilitating microbial interactions of interest to the Department of Energy and other clients.

CURRENTLY FUNDED PROJECTS IN THE CHEMICAL IMAGING INITIATIVE

Light-Source-Based Imaging

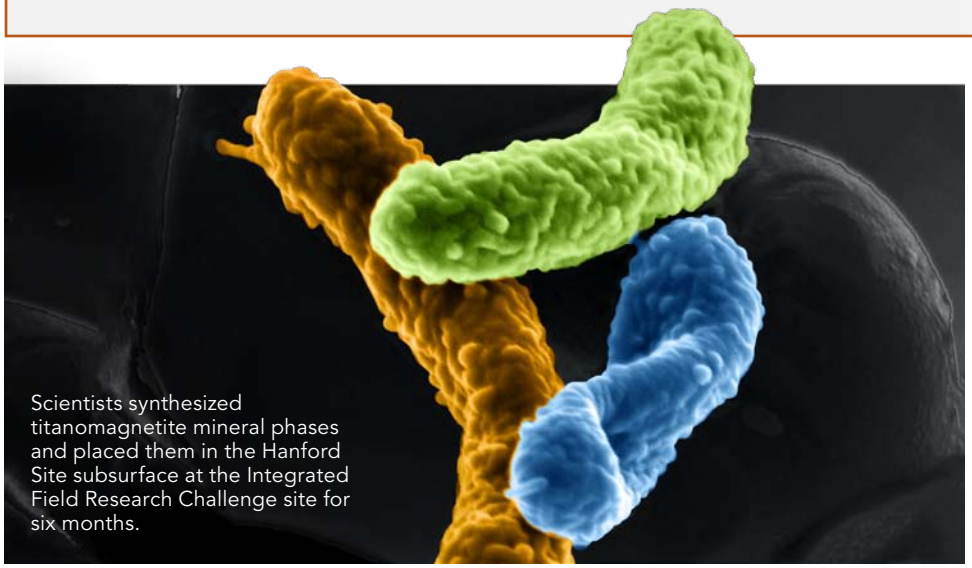
- Correlative High-Resolution Imaging and Spectroscopy to Characterize the Structure and Biogeochemical Function of Microbial Biofilms. *Principal Investigator: Dr. Matthew Marshall*
- Integrated Nano-Scale Imaging for Investigating Applications and Implications of Nanomaterials. *Principal Investigator: Dr. Galya Orr*
- Chemical Imaging Analysis of Environmental Particles. *Principal Investigator: Dr. Alexander Laskin*

Multimodal Analysis and Integration Framework for Chemical Imaging

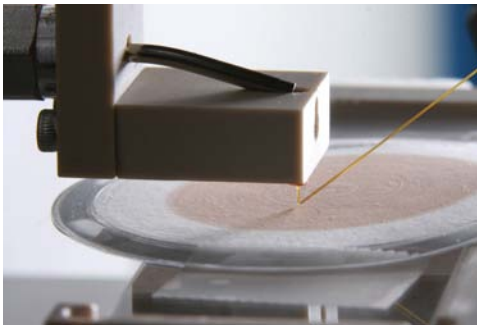
- A Multimodal Integration Framework for Chemical Imaging. *Principal Investigator: Dr. Kerstin Kleese van Dam*
- Synergistic Integration of Feature Recognition and Analysis for Chemical Imaging Data. *Principal Investigator: Dr. James Carson*

In-House Imaging

- Site-Specific Atomic-Resolution Probing of Structure-Property Relationship under Dynamic and/or Operando Conditions using *In Situ* and *Ex Situ* Chemical Imaging Based on Multi-Instrument Approach. *Principal Investigator: Dr. Chongmin Wang*
- Development of New Soft Ionization Mass Spectrometry Approaches for Spatial Imaging of Complex Chemical and Biological Systems. *Principal Investigator: Dr. Julia Laskin*
- Facet-Specific Chemistry of Nanoscale Crystalline Alumina Using an Enhanced Scattering Infrared Near-Field Optical Microscope. *Principal Investigator: Dr. Scott Lea*



Scientists synthesized titanomagnetite mineral phases and placed them in the Hanford Site subsurface at the Integrated Field Research Challenge site for six months.



A new soft ionization mass spectrometry approach is being developed for spatial imaging of complex chemical and biological systems of interest in energy production and environmental cleanup.

About the Chemical Imaging Initiative

At Pacific Northwest National Laboratory, initiatives are designed to build new capabilities that can advance scientific frontiers and solve problems for our clients. Through interdisciplinary teams, the Chemical Imaging Initiative will deliver new imaging tools and capabilities in nanometer-scale and element-specific imaging. We are seeking scientific and industrial partnerships for these activities in the 5- to 7-year timeframe.

About Pacific Northwest National Laboratory

Pacific Northwest National Laboratory is a Department of Energy Office of Science national laboratory where interdisciplinary teams advance science and technology and deliver solutions to America's most intractable problems in energy, the environment and national security. PNNL employs approximately 4,900 staff, has an annual budget of nearly $1.1 billion, and has been managed by Ohio-based Battelle since the lab's inception in 1965. Follow PNNL on Facebook, LinkedIn and Twitter.

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April 2011 PNNL-SA-79318