EMSL: Scientific *Integration*. Scientific *Innovation*. Scientific *Impact*.

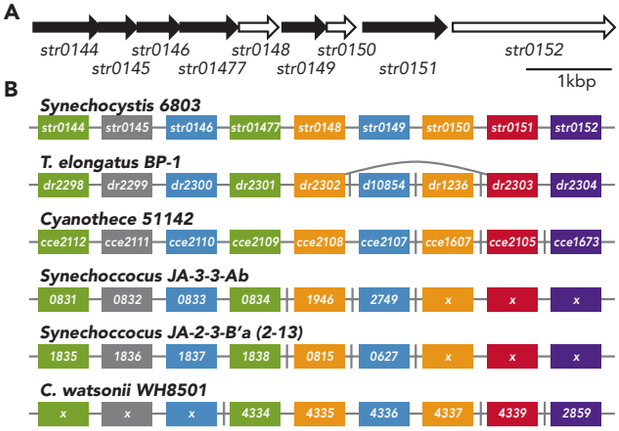
EMSL develops and integrates world-leading capabilities that transform the scientific community's understanding in the environmental molecular sciences and accelerate discoveries and innovation relevant to DOE's missions. These scientific advances are accomplished through strong, multidisciplinary collaborations between an engaged user community and expert scientists at EMSL. Examples from EMSL's research portfolio, which is focused on three Science Themes, exemplifies the scientific impact enabled by EMSL in research important to DOE and the nation.

BIOLOGICAL INTERACTIONS AND DYNAMICS

On the Light Path to Bioenergy: High-sensitivity proteomics leads to discovery of operon in O_2-producing protein.

Future clean energy will rely heavily on efficient conversions of light energy into biofuel. Researchers from PNNL and Washington University in St. Louis discovered a novel cluster of genes that encode proteins essential for green plants to thrive. They identified six proteins linked to a complex called photosystem II (PSII), which forms a cluster of nine genes. This research can lead to a better understanding of how these proteins work in other electron transport chain mechanisms, which could alter how we view photosynthesis.

KM Wegener et al., *Journal of Biological Chemistry* 283(41):27829-27837



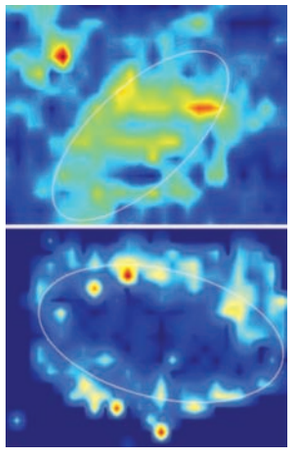
Representation of the operon in (A) Synechocystis 6803 and (B) other cyanobacteria. In A, the black arrows indicate open reading frames whose products were observed to be differentially expressed in PSII complexes isolated from various mutant strains. In B, the slash indicates genes are not clustered. X indicates that there is no ortholog, or similar gene, in the genome. The numbers correspond to the gene designation or contig number in various cyanobacteria.

GEOCHEMISTRY/BIOGEOCHEMISTRY AND SUBSURFACE SCIENCE

Tips for Nanomapping: Atomic force microscopy technique maps proteins on Shewanella surface.

An international team used a combination of surface science and imaging capabilities to determine, with nanoscale resolution, the location, of two *Shewanella oneidensis* MR-1 surface proteins (MtrC and OmcA) that can affect environmental quality. Bacteria such as *Shewanella* exchange electrons with minerals, yielding effects such as changes in the migration of environmental contaminants and water purity. EMSL's imaging capabilities offered a deeper understanding of the role MtrC and OmcA play in electron exchange, which may lead to enhanced bioremediation methods for contaminated environments.

BH Lower et al., *Applied and Environmental Microbiology* 75(9)2931-2935



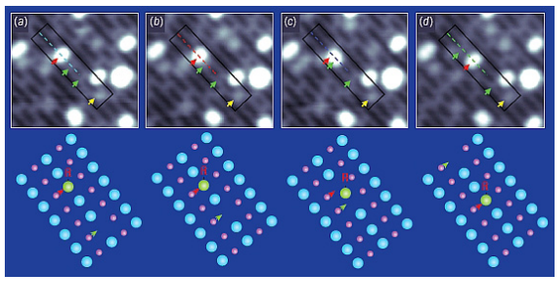
Antibody-recognition force microscopy was used to map MtrC and OmcA on the Shewanella surface. This work was featured on the cover of Applied and Environmental Microbiology.

SCIENCE OF INTERFACIAL PHENOMENA

Alcohol Exploits Defects to Its Advantage: Scientists unlock mystery of how alcohol splits, travels on surface of catalyst.

The combination of EMSL unique scanning tunneling microscopy and Chinook supercomputer allowed PNNL users to discover how alcohol molecules behave on the surface of a common catalyst like titanium oxide. Their discovery could help them tailor molecular delivery systems, leading to the development of new, clean energy sources and the design of technologies that use titanium dioxide, such as air and water purifiers.

Z Zhang et al., *Physical Review Letters* 101:156103



Images from a scanning electron microscope (top) and a simple model show how the oxygen from the alcohol (green with R on top) diffuses on the surface of titanium dioxide (the oxygen is represented by the blue spheres and the titanium by the purple).

ABOUT EMSL

EMSL—the Environmental Molecular Sciences Laboratory—a U.S. Department of Energy national scientific user facility 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.

Sponsor: The U.S. Department of Energy's Office of Biological and Environmental Research

Year opened: 1997

Annual operating cost: ~$35 million

Resident scientists: Nearly 250

Staff and user recognition (past 3 years):

- EO Lawrence Award
- Three Presidential Early Career Award for Scientists and Engineers
- Fellowships in NAS, AVS, AAAS, MRS, and APS.

User community: nearly 700 annually from all 50 states and nearly 40 countries.

Scientific impact: Nearly 1000 publications, more than 30 journal covers, and 6 patents in the past three years.

EMSL:

- World's first solids/liquids-capable 900-MHz NMR spectrometer
- One of the first 12-tesla magnets for FTICR mass spectrometry—enabling top-down proteomics
- DOE's first highly scalable computational chemistry software, NWChem.

UNPARALLELED CAPABILITIES

EMSL houses an unparalleled collection of state-of-the-art capabilities that are used to address scientific challenges relevant to DOE and the nation. Researchers from around the world are encouraged to use EMSL's unique capabilities with an emphasis on merging computational and experimental instruments. These capabilities evolve with the needs of EMSL users, such that they are upgraded over time and customized as necessary. To save users time and cost, EMSL's supercomputer and NMR resources can be accessed remotely.

Cellular Isolation and Analysis

Isolating cells from environmental samples provides a foundation for understanding the dynamics of microbial communities; coupled with cutting-edge imaging, genomics, and proteomics analyses, cellular isolation and analysis tools enable a new field of systems biology.

Subsurface Flow and Transport

Users apply subsurface flow and transport tools at EMSL, focusing on the application of fundamental physical chemistry concepts to the study of chemical reactions in heterogeneous natural materials, with an emphasis on soil and subsurface systems.

Molecular Science Computing

Chinook, EMSL's high-performance, massively parallel supercomputer; premiere computational chemistry software, NWChem; and graphics and visualization tools advance a wide range of experimental activities in environmental molecular research—such as benchmark calculations on small molecules, reliable calculations on large molecules and solids, simulations of large biomolecules, and reactive chemical transport modeling.

Mass Spectrometry

Unmatched mass spectrometry capabilities at EMSL allow high-throughput, high-resolution analysis of complex systems and can be applied to scientific problems ranging from proteomics studies to aerosol particle characterization, as well as fundamental studies of ion-surface collisions and preparatory mass spectrometry using ion soft-landing.

Microscopy

EMSL's imaging tools offer nanoscale–and even atomic–resolution of a vast range of sample types with applications to surface, environmental, biogeochemical, atmospheric, and biological science.

Deposition and Microfabrication

Users can tailor surfaces, atom by atom, with an emphasis on oxide mineral films and interfaces, ranging from high-quality, single-crystal thin films to nanostructures with EMSL's deposition and microfabrication tools.

NMR and EPR

To advance interfacial and *in situ* chemistry and biology, environmental chemistry, metallocomplex research, and more, EMSL offers users NMR tools ranging from a 300-MHz magnet to a powerful, and first-of-its-kind 900-MHz NMR magnet, as well as a variety of sophisticated probes and techniques.

Spectroscopy and Diffraction

Remarkable resolution is achieved with EMSL's wide array of spectroscopy and diffraction tools that enable users to study solid-, liquid-, and gas-phase sample structure and composition.

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To submit a proposal for use of EMSL, or to learn more about the science conducted at EMSL and the instruments and expertise available to users, visit www.emsl.pnl.gov.

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