EMSL

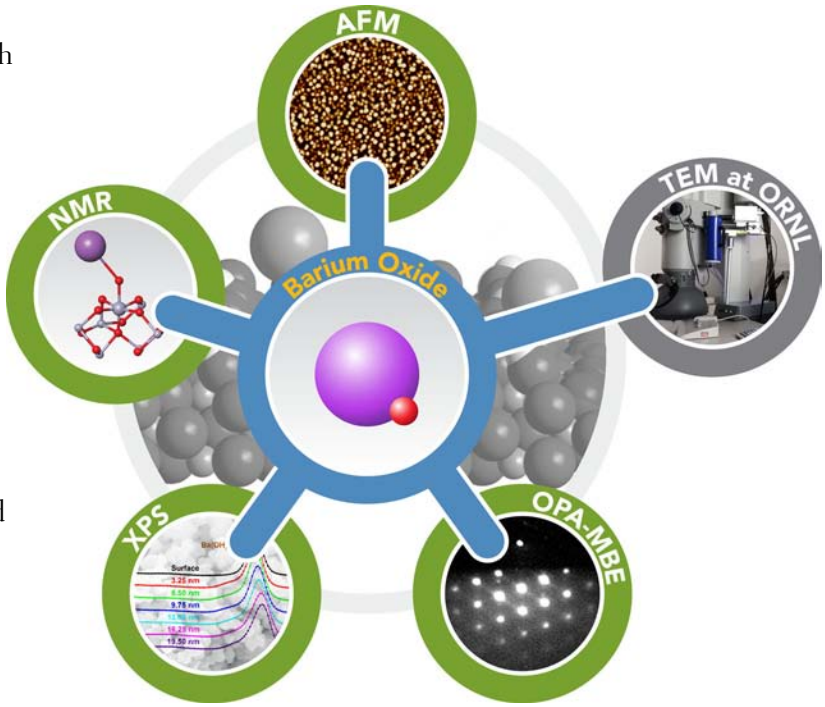
Change Your Perspective: Integrate EMSL into Your Research

Integration and collaboration are cornerstones of research at EMSL—the Environmental Molecular Sciences Laboratory, a U.S Department of Energy national scientific user facility on the Pacific Northwest National Laboratory campus in Richland, Washington. Expand your surface and interface research tool box by integrating EMSL's wealth of state-of-the-art and unique experimental instruments and advanced capabilities in atomistic computation. Exchange ideas and customize your experiments through collaborations with our expert staff in an environment designed to foster problem-solving. Your EMSL experience will give you a fresh perspective that will foster innovative solutions to the scientific problems you study related to energy and the environment.

ONE LOOK AT INTEGRATION AND COLLABORATION AT EMSL

EMSL researchers are taking pollution prevention to a new level – the atomic level, that is. Barium oxide (BaO) grabs and stores nitrogen oxide (NO_x), holding promise for emissions control. EMSL capabilities allowed researchers to study BaO catalysts from many angles, including how BaO nanoparticles form, BaO nanoparticle characteristics on an yttria-stablized zirconia (YSZ) support, and BaO binding on an aluminum oxide (Al_2O_3) support. This rounded characterization was made possible by the full spectrum of traditional and non-traditional surface science capabilities under the EMSL roof, including:

- 900-MHz nuclear magnetic resonance (NMR) to identify the penta-coordinated reactive Al site
- Oxygen-plasma-assisted molecular beam epitaxy (OPA-MBE) for high-quality BaO thin-film growth
- High-resolution infrared spectroscopy (IR) measurements to identify the vibrational modes
- *ex-situ* high-resolution x-ray diffraction (XRD) for structural analysis
- *in-situ* high-resolution transmission electron microscopy (HR-TEM) to investigate the morphological and chemical state changes under reaction conditions
- High-resolution x-ray photoelectron spectroscopy (XPS) to identify the chemical state of elements.



One system, multiple analyses. Researchers applied different approaches using capabilities at EMSL and collaborating institutions to study a BaO catalyst system.

Collaborative participants in these ongoing studies include researchers from PNNL; Oak Ridge National Laboratory, Tennessee; Hanbat National University, Taejon, Korea; and Nanjing Normal University, Nanjing, China.

See the full set of available EMSL tools that might be applied to your research at www.emsl.pnl.gov/capabilities.

Kwak *et al.* 2007. "Penta-Coordinated Al^{3+} Ions as Preferential Nucleation Sites for BaO on γ-Al_2O_3: An Ultra-High-Magnetic Field ^{27}Al MAS NMR Study." *Journal of Catalysis* 251:189-194.

Nachimuthu *et al.* 2009. "Growth and Characterization of Barium Oxide Nanoclusters on YSZ(111)." *Journal of Physical Chemistry C* 113 (32): 14324-14328.

ABOUT EMSL

EMSL, a U.S. Department of Energy national scientific user facility located 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.

EMSL's distinctive focus on integrating computational and experimental capabilities as well as collaborating among disciplines yields a strong, synergistic scientific environment. Bringing together experts and an unparalleled collection of state-of-the-art instruments under one roof, EMSL has helped thousands of researchers use a multidisciplinary, collaborative approach to solve some of the most important and complex national scientific challenges in energy and environmental sciences.

To learn more about EMSL, the science conducted at EMSL, as well as the instruments and expertise available to users, visit www.emsl.pnl.gov.

BECOME AN EMSL USER

Researchers are invited to access the world-class capabilities and collaborate with the internationally recognized experts at EMSL via its peer-reviewed proposal process. To submit a proposal, follow the five-steps outlined on the EMSL website (www.emsl.pnl.gov) under User Access. Current and potential EMSL users are encouraged to respond to Calls for Proposals, which are announced each spring. However, unique research proposals that fall outside the Calls for Proposal focus may be submitted at any time.

Applicants are encouraged to submit proposals for use of EMSL's capabilities with an emphasis on integrating computational and experimental tools. In general, users whose open research proposals are accepted may use EMSL resources free of charge. Open research is loosely defined as science and engineering research for which the resulting information is published and shared broadly within the scientific community.

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NEW DECADE, NEW TOOLS, NEW SCIENCE

EMSL evolves with the needs of its scientific users, and this evolution is being accelerated by the American Recovery and Reinvestment Act. EMSL is expanding its capability sets that can be applied to surface science studies, acquiring a new generation of tools that will enable materials development and characterization in the next decade. Capabilities that are on the way include:

High-Spatial Resolution Capabilities

3D-Atom probe tomography: 0.2-nm resolution and part-per-million sensitivity

Helium ion microscope: sub-nanometer imaging and ion-scattering capability

NanoSIMS: 50-nm resolution

Imaging XPS systems: ~2-µm resolution for imaging and spectra

Single-site chemistry: ~0.1-nm resolution using scanning probe microscopy combined with surface analytical capabilities.

In-situ Real-Time Capabilities

Sum frequency generation and second harmonic generation: rapid characterization of surfaces and interfaces in optically transparent environments

Environmental TEM: aberration-corrected TEM with *in situ* reaction cells for gaseous and liquid environments

Tip-enhanced IR spectroscopy: 20-nm resolution in ambient or controlled gaseous environments

Radiological Capabilities

A dedicated suite of analytical capabilities including XPS, electron microprobe, focused ion beam/scanning electron microscope, and NMR instruments for studying systems involving radiological materials.

Synthesis of Advanced Materials

Advanced MBE system for growth of high-quality complex oxide thin films with well-controlled dopant concentrations.

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