EMSL

Capabilities Series

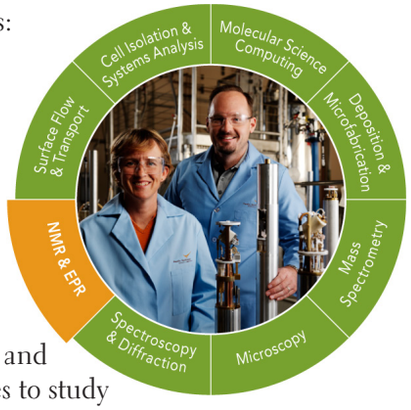
NMR and EPR

EMSL houses a suite of nuclear magnetic resonance (NMR) spectrometers with frequencies ranging from 300 to 900 MHz. To complement its NMR suite, EMSL also offers a pulsed, ELDOR-capable, 9.5-GHz electron paramagnetic resonance (EPR) spectrometer. EMSL's NMR and EPR instruments are part of an unparalleled collection of capabilities designed to support research that integrates both experimental and computational tools. When their integrated use is applied to EMSL's science themes of Biological Interactions and Dynamics, Geochemistry/Biogeochemistry and Subsurface Science, as well as Science of Interfacial Phenomena, NMR and EPR enable novel, fundamental research in:

- **Energy** – making strides toward alternative energy sources
- **Environmental research** – understanding contaminant fate and transport for the remediation of unhealthy environments
- **Catalysis** – observing catalysts at the molecular level to then tailor them for specific functions
- **Biology** – relating the structure and function of proteins with critical cellular roles
- **Capability development and integration** – enhancing spectral interpretation with computational tools and enabling new NMR measurements via novel capabilities.

CAPABILITY DETAIL

EMSL offers scientific users:



- NMR for high-field liquid- and solid-state measurements
- Extreme-temperature NMR probes, including high-temperature probes to observe catalysts in their near-native states and low-temperature probes to study metalloprotein chemistry and structure
- A novel BioMAS/900-MHz system for high-resolution and ultrahigh-field bio-solid studies
- NMR with metabolomics capabilities to identify and quantify metabolites in complex biofluids
- NMR with radiological capabilities
- Combined confocal microscopy and NMR
- Pulsed EPR for studying the structure and conformational changes of biomolecules and biocomplexes that do not lend themselves to study by x-ray diffraction and NMR techniques.

WHY NMR AT EMSL?

- EMSL provides NMR and EPR tools as well as staff expertise within the context of an integrated problem-solving environment.
- In-house, custom probe design and development is a specialty at EMSL.
- Many of EMSL's NMR spectrometers can be accessed remotely, allowing users to control these world-class instruments from their home institutions.
- Customization of NMR tools, such as for metabolomics studies, provides EMSL users with unmatched research opportunities.

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.pnnl.gov.

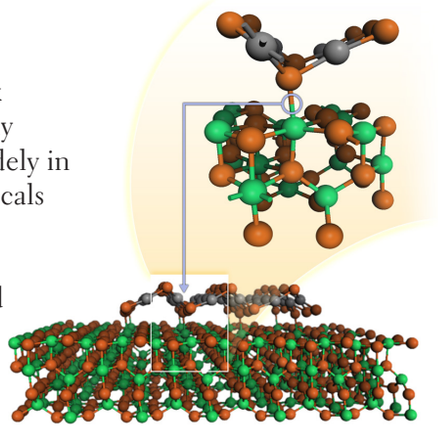
BECOME AN EMSL USER

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.pnnl.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, most 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.

NMR RESEARCH HIGHLIGHTS

Catalytic Catamarans: Preventing Pollution



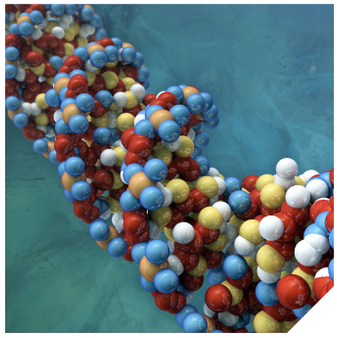
Rafts of catalytic platinum oxide float above a sea of aluminum oxide, anchored by bonds between platinum and aluminum.

EMSL's 900-MHz NMR and Chinook supercomputer were integrated to study platinum catalysts—materials used widely in industry for petroleum refining, chemicals production, and pollution prevention. Employing ultrahigh-field NMR, researchers attained an unprecedented molecular-level view of Pt binding to an aluminum oxide (Al_2O_3) support. These experimental data were combined with theoretical calculations to yield a model of how rafts of Pt oxide are formed and anchored to the surface of Al_2O_3, providing fundamental insight on where catalytic reactions occur. The team's findings were published in *Science*, and could help engineers optimize such rafts to develop more efficient, less costly catalysts.

EMSL Users: Pacific Northwest National Laboratory, Oak Ridge National Laboratory, and Sungshin Women's University

Kwak et al. 2009. *Science* 325(5948):1670-1673.

A Hairpin Turn: Optimizing Antivirals



With the help of NMR, EMSL users have developed a rational, structure-based method for designing and optimizing antiviral peptides. Using HIV-1 as a system of study, the team focused on the virus's Tat-TAR binding site, a protein-RNA interaction essential to HIV-1 replication. The team tested approximately 100 peptides, or Tat mimics—each built as a closed circle with a β-hairpin loop on one end such that it would nestle snugly into the TAR binding site for Tat, disrupting the Tat-TAR interaction—and three stood out from the crowd for their notable potency. The team's successful results with HIV-1, reported in the *Proceedings of the National Academy of Sciences*, give reason to be optimistic that the approach will be adaptable for a wide range of viral strains.

EMSL Users: University of Washington, the University of Zurich, and Case Western Reserve University

Davidson et al. 2009. *Proceedings of the National Academy of Sciences* 106(29):11931–11936.

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