



# Molecular Science Computing

The Molecular Science Computing capability at EMSL provides users with an integrated production computing environment that includes advanced high-performance computing resources, EMSL-wide data storage, and expert staff critical to support world-class fundamental research with the increasingly predictive, system-level simulation tools required to address complex environmental molecular science challenges. Solving intricate scientific problems requires multidisciplinary science, including close integration of cutting-edge experiments and simulations, instantaneous data access, and essential analysis and visualization capabilities. The integration of EMSL's advanced instrumentation and computational techniques are part of an unparalleled collection of capabilities designed to enable unique cross-discipline research into core Science Themes—Biological Interactions and Dynamics, Geochemistry/Biogeochemistry and Subsurface Science, and Science of Interfacial Phenomena. EMSL's Molecular Science Computing capability supports a wide range of activities in environmental molecular research, including:

- ▶ Molecular-scale chemical processes such as catalysis modeling, hydrogen production and storage modeling, simulation of material and surface properties and nanoparticles, study of complex biomolecular systems and interactions, solution chemistry, and the behavior of heavy elements in the environment
- ▶ Bioinformatics and computational biology modeling, which analyzes large experimental data sets to obtain a systems-level view of biological processes in living cells
- ▶ Subsurface reactive flow and transport modeling and cloud/aerosol modeling to monitor climate change.

## CAPABILITY DETAIL

### Computing Systems

- ▶ Chinook supercomputer consisting of 18,480 processor cores with a theoretical peak performance of 163 teraflops, 74 terabytes of memory, 1.25 petabytes of fast local and global disk space with an aggregate bandwidth of 1 terabyte per second, and a fast Infiniband Interconnect
- ▶ Aurora data archive connected to the supercomputer and experimental capabilities at EMSL, delivering 4.5 petabytes of storage capacity
- ▶ Graphics and Visualization Laboratory for analysis and high-end visualization of complex experimental and computational data sets with image, audio, and video capabilities.



### Scientific Consultants

- ▶ In-house personnel to assist with setting up computer simulations, trouble-shooting, installing or optimizing software, designing simulations, and scientific data analysis
- ▶ Native language assistance for Chinese users, including Mandarin.

### Scalable Software

- ▶ EMSL's Molecular Science Software Suite, consisting of NWChem, Extensible Computational Chemistry Environment (Ecce), and the Global Array Toolkit, provides an integrated set of tools that enables scientists to understand complex chemical systems at the molecular level by coupling the power of advanced computational chemistry techniques with existing and rapidly evolving high-performance, massively parallel computing systems
- ▶ ScalaBLAST is a parallel, high-performance Basic Local Alignment Search Tool engine for performing whole-genome or multiple-genome BLAST calculations against a variety of databases
- ▶ Support for various commercial and open-source software packages can be found in the Molecular Science Computing capability section on the EMSL website.



## WHY USE EMSL'S MOLECULAR SCIENCE COMPUTING CAPABILITY?

- ▶ Molecular Science Computing provides users with an integrated suite of computing hardware and software capabilities optimized for achieving the fastest time-to-solution for complex systems-level environmental molecular science simulations.
- ▶ Expert staff members have extensive knowledge and experience in high-performance computing, as well as the operations, domain expertise, and scientific knowledge to support EMSL's users.
- ▶ Substantial integration of transformational high-end computing simulations with experimental resources at EMSL provides a unique multidisciplinary research environment.

## 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](http://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](http://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, 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.

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## MOLECULAR SCIENCE COMPUTING RESEARCH HIGHLIGHTS

### *Silver Helps Make Propylene Oxide a Better Commodity*

Propylene oxide is a key precursor for the production of commodity chemicals, including household detergents, plastics, and paints. The current methods available to produce industrial-scale propylene oxide are expensive or environmentally unfriendly due to the chlorinated or peroxy-carboxylic waste byproducts.

Scientists, led by a team from Argonne National Laboratory, conducted periodic, self-consistent density functional theory (DFT) calculations using EMSL's Molecular Science Computing capability as part of an experiment to determine how unpromoted, size-selected silver trimer ( $\text{Ag}_3$ ) clusters and ~3.5-nanometer silver nanoparticles on alumina supports can catalyze propylene epoxidation with only a negligible amount of carbon dioxide formation and still maintain high activity at low temperatures. The DFT calculations conducted at EMSL, which were based on a plane-wave basis set using the Vienna ab initio simulation package (VASP), revealed that oxidized silver trimers are more active and selective for epoxidation because of the open-shell nature of their electronic structure. The results suggest new architectures based on ultra-small silver particles may provide highly efficient catalysts for propylene epoxidation, potentially expanding their applications to other systems.

EMSL Users: Argonne National Laboratory; Fritz-Haber-Institut der Max-Planck-Gesellschaft, Department of Inorganic Chemistry; and the University of Illinois at Chicago. Lei et al. 2010. *Science* 328(5975):224-228. DOI: 10.1126/science.1185200.

### *Researchers Take a New Look at Azurin by Integrating EMSL's Supercomputing and Spectroscopy Capabilities*

Metalloproteins, such as the copper-containing azurin, play a major role in catalyzing electron transfer in cellular reactions. Previously, copper's large nuclear quadrupole interactions produced weak nuclear magnetic resonance signals. However, scientists from Pacific Northwest National Laboratory and the University of Nebraska obtained the first high-field nuclear magnetic resonance signal of a copper site in a copper protein by integrating EMSL's 800-MHz nuclear magnetic resonance spectrometer with the Chinook supercomputer. This allowed the scientists to perform previously impossible experiments and validate the results with powerful calculations and models. The team used these advances to complete azurin's data pool, finding informative spin-lattice relaxation of samples unexpectedly efficient even when using 800-MHz nuclear magnetic resonance. Then, data were reproduced using theoretical calculations, confirming details of the electronic structure. The technique turned the quadrupolar nature of azurin into an advantage, and the researchers gained a sensitive measure of the electron density around the nuclear site that revealed previously unknown details about the electronic structure and environment of azurin's copper center.

EMSL Users: Pacific Northwest National Laboratory Biological Sciences Division and University of Nebraska Department of Chemistry.

Lipton et al. 2009. *Journal of the American Chemical Society* 131(39):13992-13999. DOI: 10.1021/ja901308v.



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