William R. Wiley
Environmental Molecular Sciences Facility

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) national scientific user facility. EMSL is the centerpiece of DOE's commitment to provide world-class research capabilities for enabling fundamental research on the physical, chemical, and biological processes that underpin critical scientific issues.

EMSL capabilities are used to address the fundamental science that will be the basis for finding solutions to national environmental issues such as cleaning up contaminated areas at DOE sites across the country and developing "green" technologies to reduce or eliminate future pollution production. The capabilities also are used to further our understanding of global climate change, environmental issues relevant to energy production and use, and health effects resulting from exposure to contaminated environments.

If you are interested in collaborating with our scientists or using the facility's resources, more information and specific procedures for becoming an EMSL user can be found at our web site http://www.emsl.pnl.gov.

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Related Web Sites

MSCF
http://mscf.emsl.pnl.gov

EMSL
http://www.emsl.pnl.gov

TM&S
http://www.emsl.pnl.gov:2080/homes/tms/

MS^3
http://mscf.emsl.pnl.gov/capabs/mscf/software/ms3.html

Ecce
http://www.emsl.pnl.gov/pub/docs/ecce

NWChem
http://www.emsl.pnl.gov/pub/docs/nwchem

ParSoft
http://www.emsl.pnl.gov/pub/docs/parsoft

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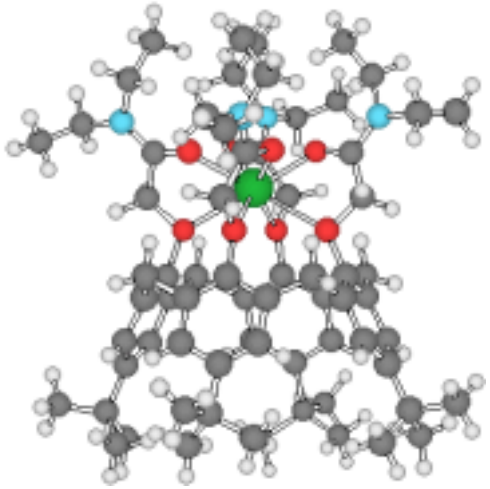

Pacific Northwest National Laboratory
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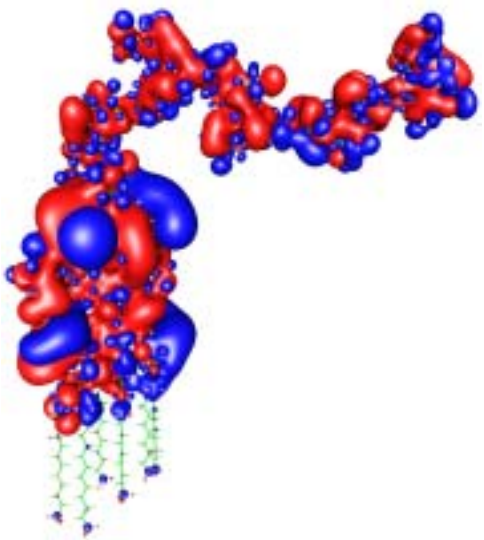

Theory, Modeling & Simulation

Theoretical and computational molecular science plays a critical role in understanding the molecular processes in many areas that are important in environmental restoration and waste management efforts. Examples of these areas include:

- migration and reactions of contaminants in soils and groundwater
- design of new ligating agents for separation of radionuclides
- tropospheric oxidation chemistry and aerosol formation
- development of environmentally benign chemical processes including catalyst design
- development of improved materials for waste storage
- enzymatic reactions involved in biodegradation of contaminants and the interaction of toxins with living organisms.

The mission of the Theory, Modeling and Simulation (TM&S) Directorate is to use computational molecular science as an aid in solving environmental problems facing the U.S. Department of Energy (DOE) and the nation. This effort combines elements from theoretical and computational chemistry, materials science, and molecular biology with computer science, applied mathematics, and advanced computing technologies. The goal is to provide a molecular-level understanding of processes in natural and contaminated environments, processes for remediating these environments, and processes that minimize further contamination of the environment. This research focuses on the environmental, energy, and other missions of the DOE, including basic science.

Molecular Science Research

Researchers in the TM&S Directorate use state-of-the-art methods to help find solutions of important environmental problems and to develop new theoretical methods and modeling and simulation techniques.

The program combines studies of fundamental molecular processes in model systems with efforts devoted to the simulation of complex multicomponent, multiphase molecular systems. Focused research efforts are underway in the following areas.

- *Computational Biochemistry, Biophysics, and Biology (CB^3).* Research focused on the development and application of computational methods for the understanding of the relationship between sequence, structure, function and dynamics of biological systems. Areas include biomolecular simulations including molecular dynamics, network analysis including kinetic simulations, and bioinformatics including genome and proteome analysis.
- *Computational Structure and Reactivity.* Apply computational methods for thermodynamics, kinetics, aqueous metal ion chemistry, ligand design, catalyst design and modeling, actinide chemistry, tank waste processing chemistry, and geochemical solid-state systems.
- *Molecular Theory and Modeling.* Develop and apply methods to understand elementary molecular processes in both the gas and condensed phases with a focus on solution chemistry and the liquid-liquid and liquid-solid interfaces.

Researchers in the TM&S Directorate also play an important role in leading and developing the Virtual Biology Facility under the Biomolecular Networks Initiative at Pacific Northwest National Laboratory, as well as in the Computational Sciences and Engineering Initiative.

Molecular Science Computing Facility

The computing demands of TM&S research programs as well as those of EMSL users are substantial and are growing dramatically as more complex problems are addressed at higher levels of accuracy. To support these efforts, the Molecular Science Computing Facility (MSCF), consisting of the High Performance Computing Center, the Graphics and Visualization Laboratory, the Experimental Computing Laboratory, and the Molecular Science Software Suite, has been established.

- The *High Performance Computing Center* supports large-scale molecular computations and includes an IBM SP 512-processor computer (247 gigaflops, 262 gigabytes of memory, and 5-terabytes disk), a Linux cluster, and a 20-terabyte data storage system as well as 2 smaller SMP-based IBM MPP computer systems used in part to evaluate promising new technologies and develop new software.
- The *Graphics & Visualization Laboratory* supports the analysis of complex molecular data and preparation of presentation materials.

The MSCF is a national scientific user resource. Access to the facility can be gained by submitting a proposal. The proposal process is described at the following web site: http://www.emsl.pnl.gov/pub/docs/tms/mscf/proposals/. Once a proposal has been accepted and access is gained, an Operations Group and a Visualization and User Services Group support MSCF users.

Molecular Science Software Suite

MS^3 is a winner of the 1999 R&D 100 Award and the 2000 Federal Laboratory Consortium Award for Technology Transfer. The EMSL-developed software suite is composed of the Extensible Computational Chemistry Environment *Ecce*, the Northwest Computational Chemistry Software *NWChem*, and The Parallel Software Development Tools *ParSoft*. The software is developed and supported by the Molecular Science Software group.