

Chinook @ EMSL

Kevin Regimbal (kevin.regimbal@pnl.gov)

Program Manager

Molecular Science Computing

EMSL's Mission

EMSL, a 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.



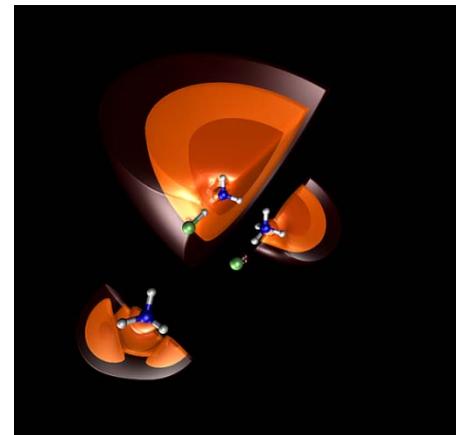
Environmental Molecular Sciences Laboratory: A National Scientific User Facility



Capabilities

EMSL houses an unparalleled collection of state-of-the-art capabilities that are used to address scientific challenges:

- **Molecular Science Computing**
- Cell Isolation and Systems Analysis
- Deposition and Microfabrication
- Mass Spectrometry
- Microscopy
- NMR and EPR
- Spectroscopy and Diffraction
- Subsurface Flow and Transport



Scientific Insight



Science Themes

Capabilities are available to users, generally at **no cost** to the user, for research in three science themes:



Biological Interactions and Dynamics

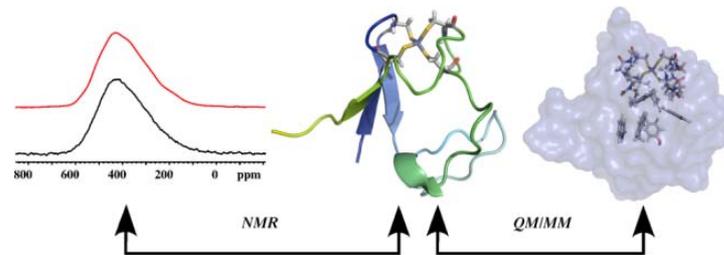


Geochemistry/Biogeochemistry and Subsurface Science



Science of interfacial Phenomena

Integrating Modeling and Experiment



EMSL also provides software to enable scientific research. The **Molecular Science Software Suite** is comprised of three packages:



MS³

MOLECULAR SCIENCE
SOFTWARE SUITE



NWCHEM

HIGH-PERFORMANCE COMPUTATIONAL
CHEMISTRY SOFTWARE

Computational chemistry software suite designed to perform Quantum and Classical Mechanics calculations on parallel supercomputers



GA TOOLS

PARALLEL COMPUTING LIBRARIES
AND SOFTWARE TOOLS

Efficient and portable shared-memory programming interface for distributed-memory computers



ECCE

EXTENSIBLE COMPUTATIONAL
CHEMISTRY ENVIRONMENT

Graphical user interface, scientific visualization tools, and underlying data management framework

Proposal Types

- **General** (anytime)
- **Science Theme** (Call for Proposals in Spring for October 1 awards)
- **Computationally Intensive Research** (Call of Proposals in Spring for October 1 awards)
- **Partner Proposal Call** (anytime)



Collaborating to build Capability

The objective of the partner program is to facilitate the development of unique capabilities in support of environmental molecular science.



Becoming an EMSL User

Proposal Process

- 1 **Contact** an EMSL staff member
- 2 **Submit** a proposal via the EMSL User Portal
- 3 **Stand by** while your proposal is processed
- 4 Visit EMSL or **arrange remote use**
- 5 **Close out**

Visit EMSL's Website:

<http://www.emsl.pnl.gov/access>



Yong Wang, EMSL User
Pacific Northwest National Laboratory



Alexis Templeton, EMSL User
University of Colorado



Claire Johnson, EMSL User
University of Washington

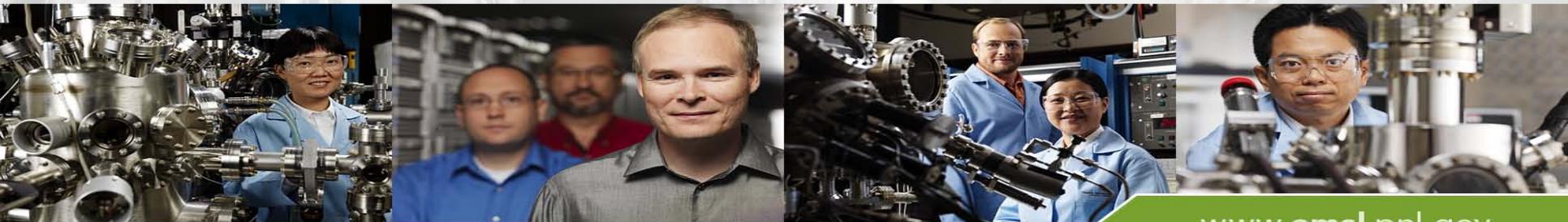


Questions



Environmental Molecular Sciences Laboratory

A national scientific user facility integrating experimental and computational resources for discovery and technological innovation



www.emsl.pnl.gov

