Research Resources for Subsurface Science

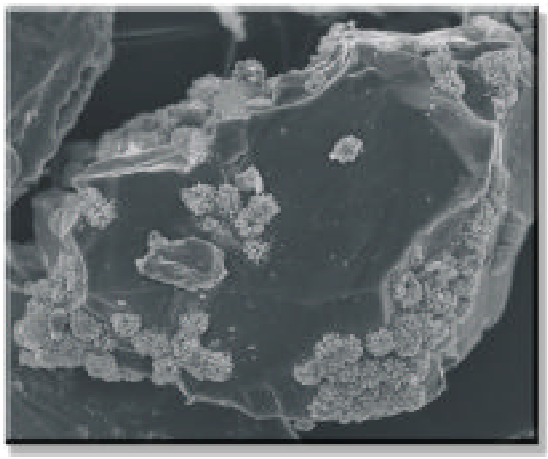
The **William R. Wiley Environmental Molecular Sciences Laboratory** (EMSL) is a U.S. Department of Energy (DOE) National Scientific User Facility at the Pacific Northwest National Laboratory in Richland, Washington, and is supported by DOE's Office of Biological and Environmental Research. EMSL was opened for use in 1997 and houses more than 100 experimental systems for molecular science, including a massively parallel super computer and the world's highest field (11.5 T) Fourier transform mass spectrometer. All of these resources are available to the scientific community. A primary focus of the laboratory is to closely couple experimental and computational research to yield insights not attainable by computation or experiment alone.

The EMSL was conceptualized and designed as the nation's premier facility for performing fundamental research at the molecular level in support of DOE's environmental management and remediation mission. In this regard, EMSL resources support many research disciplines in the environmental sciences, with particular emphasis on physical chemistry. Disciplines where significant staff and instrument/modeling capabilities exist include atmospheric and aerosol chemistry, soil and water chemistry, mineralogy and mineral physics, geochemistry and biogeochemistry, colloid chemistry, and environmental microbiology.

In the area of **Subsurface Science**, EMSL staff and users are now playing a key role in resolving fundamental scientific issues associated with contaminant migration at the Hanford Site through fundamental studies of model systems and investigations of contaminated materials from the field. Important EMSL resources for addressing subsurface issues include, but are not limited to:

- Comprehensive capabilities in vibrational and optical spectroscopies for characterizing the interaction of contaminants with mineral/colloid surfaces, microbes, and plant roots (mechanism, kinetics, and speciation) at the molecular and microscopic scale.
- World-class surface science laboratories for surface chemical state determination, detailed surface chemical analyses of particles from nanometers to microns, and characterization of natural particle coatings and colloids.

Analyses of Contaminated Hanford Sediment



Zeolite Clusters on Quartz Particle

Zeolite Clusters on Quartz Particle (x23,000)

- Unparalleled particle characterization facilities for determining the size, charge, structure, valence, bonding environments, thermodynamics, and other intensive properties of pristine, engineered, and contaminated geologic particles and materials. Techniques include laser light scattering, electrophoresis, microcalorimetry, X-ray diffraction, Mössbauer spectroscopy, and nuclear magnetic resonance.
- Scanning probe microscopes (atomic force and tunneling) and high resolution electron microscopes (scanning and transmission) for real time measurements of the surface and internal structure of reactive environmental particles.
- A magnetic resonance imaging facility where pore scale features, mineral density variations, fractures, water migration, and sorbate dynamics can be mapped in three dimensions in centimeter-scale cores of mineral or subsurface materials.
- A mesoscale flow cell laboratory where meter-scale reactive transport experiments may be performed and monitored directly using advanced measurement tools to evaluate the upscaling of molecular/microscopic mechanisms.
- Advanced geochemical modeling capabilities for solids, solutions, microbes, and their interactions, including quantum mechanics/molecular mechanics, molecular dynamics, surface complexation, macroscopic equilibrium/kinetic, kinetic biogeochemical, and reactive transport.
- The Molecular Science Computing Facility, a state-of-the-art computational chemistry resource consisting of a large, massively parallel computer (512 processor IBM SP), an experimental computing laboratory, a data archive system, a graphics and visualization laboratory, and the award-winning Molecular Science Software Suite. The unique, comprehensive, integrated software suite enables computational chemists to focus advanced techniques on complex chemical problems.
- The subsurface reactive transport code MCTRACKER and the code suite NWGrid/NWPhys, which includes packages for fluid-solid interactions, computational electro-magnetics, particle transport, chemistry and aerosol transport. This code suite has been used to develop grids for parts of the Hanford Site based on stratigraphic data. Significant efforts also are devoted to continued development of new and more accurate chemistry models needed to attack the many complex problems in the environmental sciences.

EMSL's resources are most effectively used for collaborative research, where users gain access to unique pieces of instrumentation or instrument clusters *and* interact with experienced staff members, who help them develop customized research strategies that take advantage of the extensive experimental and computational capabilities in the facility.

For additional information, please visit our website *http://www.emsl.pnl.gov*, or contact

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