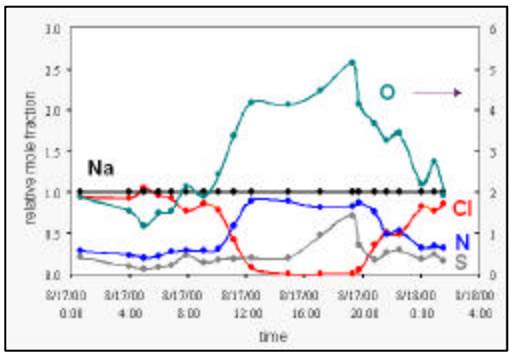
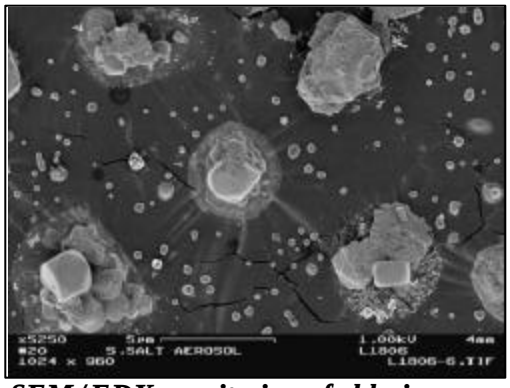
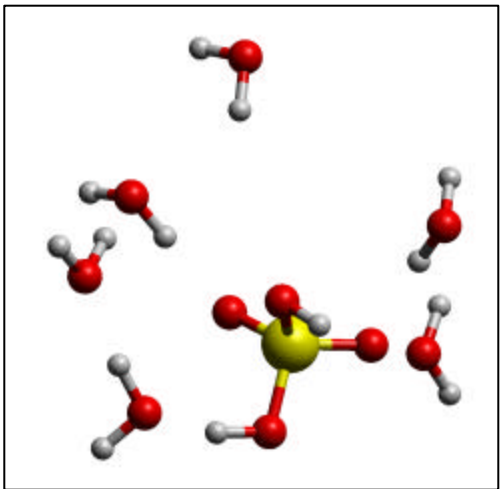
# Research Resources for Atmospheric Gas and Aerosol Chemistry



***SEM/EDX monitoring of chlorine depletion in individual sea salt particles.***



***Model of a water molecule condensing on a sulfuric acid - water cluster, which is important in the nucleation of sulfate aerosols.***

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 1998 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 gas and aerosol chemistry, soil and water chemistry, mineralogy and mineral physics, geochemistry and biogeochemistry, colloid chemistry, chemical physics and environmental microbiology.

In the area of **Atmospheric Gas and Aerosol Chemistry**, laboratory research and theoretical studies by EMSL staff and users are developing a fundamental knowledge of the chemical/physical processes of aerosols and gases that are central to addressing major air pollution issues such as climate change, human and wildlife health, quality of food and water, and visibility reduction. This involves understanding atmospheric cycling of particular chemicals, and fundamental physical properties and reaction rates of gases, aerosols, and surfaces. Key EMSL resources for identifying and characterizing important tropospheric molecules and their reactions include, but are not limited to:

**Comprehensive measurement systems for characterizing aerosols**

- automated time-resolved aerosol collector for individual particle analysis.
- elemental and mass analysis of size-segregated particles using high energy x-ray and particle beam techniques.
- a nuclear magnetic resonance facility for measuring the apportionment of organic carbon among size segregated particles.
- laser desorption ion trap mass spectrometer with single particle interface for real-time size measurements and chemical analysis of individual particles or *ex post facto* analysis of size-segregated particle samples.

**Unparalleled measurement systems for characterizing gases**

- field deployable proton transfer quadropole and ion trap mass spectrometers for trace gas detection.
- *in situ* infrared laser spectrometer for real time gas phase measurements at ultra trace levels.
- high resolution Fourier transform infrared spectrometer for measurement of infrared absorption spectra of tropospheric trace gases. These spectra extend the capability of devices such as the *in situ* infrared laser spectrometer and are fundamental to the development of next generation gas measurement devices.
- a full suite of aircraft gas detectors involving the Battelle G1 aircraft are under development that employ versions of the above instrumentation.

**Advanced capabilities for investigating fundamental chemical and physical processes critical to atmospheric chemistry**

- coupled laminar flow tube reactor/mass spectrometer and molecular theory for particle nucleation studies.
- electronic structure and rate constant calculations of reaction pathways and kinetic parameters for VOC oxidation and Hg/halide reactions.
- molecular simulations of atmospheric processes at gas/liquid and gas/solid interfaces.

**World-class surface science laboratories** for surface chemical state determination and detailed surface chemical analyses of nanometer- to micron-sized particles.

**The Molecular Science Computing Facility**
This state-of-the-art computational chemistry resource consists 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 that enables computational chemists to focus advanced techniques on complex chemical problems.

These 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 users develop customized research strategies to take advantage of the extensive experimental and computational capabilities in the facility.

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

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Operated by Battelle for the U.S. Department of Energy