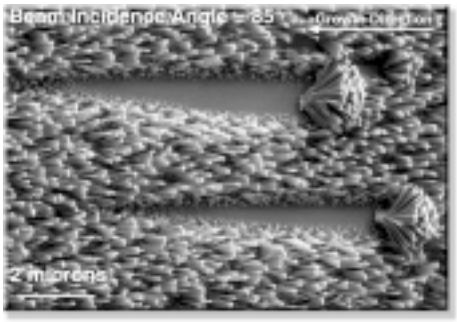
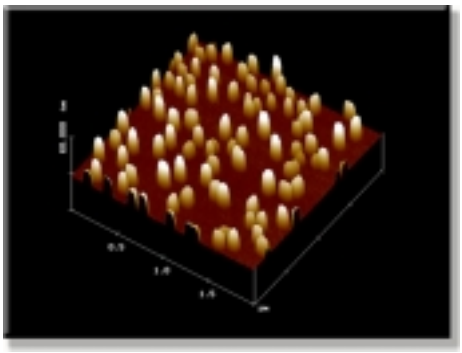
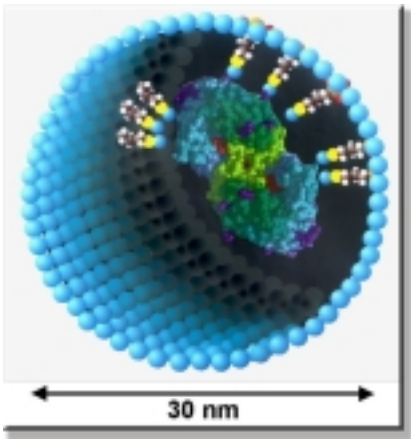
Research Resources for Nanoscale Science, Engineering, and Technology



Nanoporous MgO film, demonstrating the effect of material synthesis using a molecular beam at a high angle of incidence.



Controlled distribution of Cu_2O quantum dots on $SrTiO_3$ substrate.



Enzyme (organophosphorous hydrolase) covalently linked to nanoporous silica substrate.

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.

In the area of **Nanoscale Science, Engineering, and Technology**, EMSL staff and users pursue research activities that include studies of self-assembly processes ranging from molecules and enzymes on mesoporous substrates to formation of oxide quantum dots and highly functional nanoporous films. Unique, well-defined oxide surfaces created by molecular beam techniques and nanotube arrays created by chemical vapor deposition are being used to gain new levels of information about environmental and biological interactions at surfaces. Additionally, interfacial engineering is being used to create oxide nanostructure systems with unique properties for electronic and catalytic applications.

EMSL 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 to take advantage of the extensive experimental and computational capabilities in the facility. Important resources for nanoscale science, engineering, and technology include instrumentation and techniques for synthesizing materials with tailored nanoscale features and for characterizing materials. Additionally, EMSL's theory, modeling, and computation capabilities complement advanced experimental efforts and guide design, creation, and testing of nanoscale systems.

Synthesis

Equipment and techniques are on hand for producing and characterizing:

- **Atomic and Molecular Clusters**. Instrumentation for making clusters of various sizes, compositions, and selected energies.
- **Particles and Quantum Dots on Surfaces**. Metal and metal oxide deposition on controlled substrates for photocatalysis studies and for fabricating photonic and electronic materials.

- **Molecularly Organized Nanoscale Particles, Materials, and Composites**. Molecularly directed synthesis of ordered nanoparticles, nanoporous materials, and functional materials for environmental health, chemical, and microelectronic applications.
- **Nanotubes and Tube Arrays**. Chemical vapor deposition of hollow carbon nanotubes with controlled tube diameter and density are filled with materials on various substrates for nanosize electronic devices, catalysis, and chemical sensor applications.
- **High Dielectric Thin Films**. Metal-organic chemical vapor deposition of ultra-thin high dielectric films with conformal step coverage for CMOS gate dielectrics and DRAM capacitor applications.
- **Epitaxial Films**. Molecular beam epitaxial growth of high-quality crystalline oxide and ceramic films. Applications include electronic, magnetic, and catalytic materials.
- **Nanoporous Thin Films**. Synthesis of chemically tailored monolithic nanoporous thin films for chemical applications using molecular beam at high angle of incidence techniques.

Characterization

World-class surface science laboratories are available for determining:

- **Structure and Properties of Isolated Clusters**. Photoelectron spectroscopy for studying clusters of metals, semiconductors, and insulators.
- **Shape, Composition, and Distribution of Nanoparticles**. High-resolution auger electron microscopy (AES); scanning probe methods (AFM/STM); electron microscopy (SEM/TEM); particle size analysis.
- **Structure and Properties of Nanomaterials**. High-resolution x-ray photoelectron spectroscopy (XPS); auger electron spectrometry (AES); thin film x-ray diffraction (XRD); nuclear reaction analysis (NRA); Rutherford back-scattering (RBS); low energy electron diffraction (LEED); x-ray photoelectron diffractometry (XPD); time-of-flight secondary ion mass spectrometry (TOF-SIMS); ellipsometry.
- **Properties of Systems with Nanometer Dimensions**. For liquid environments—field flow fractionation (FFF); particle size and charge analyzers; atomic force microscopy (AFM); ultra- and super-centrifuges for separation. For "bulk" properties—x-ray diffractometry (XRD); Fourier transform infrared (FTIR) spectrometry; Mössbauer and Raman spectroscopies.

Computation

The Molecular Science Computing Facility is 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.

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

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