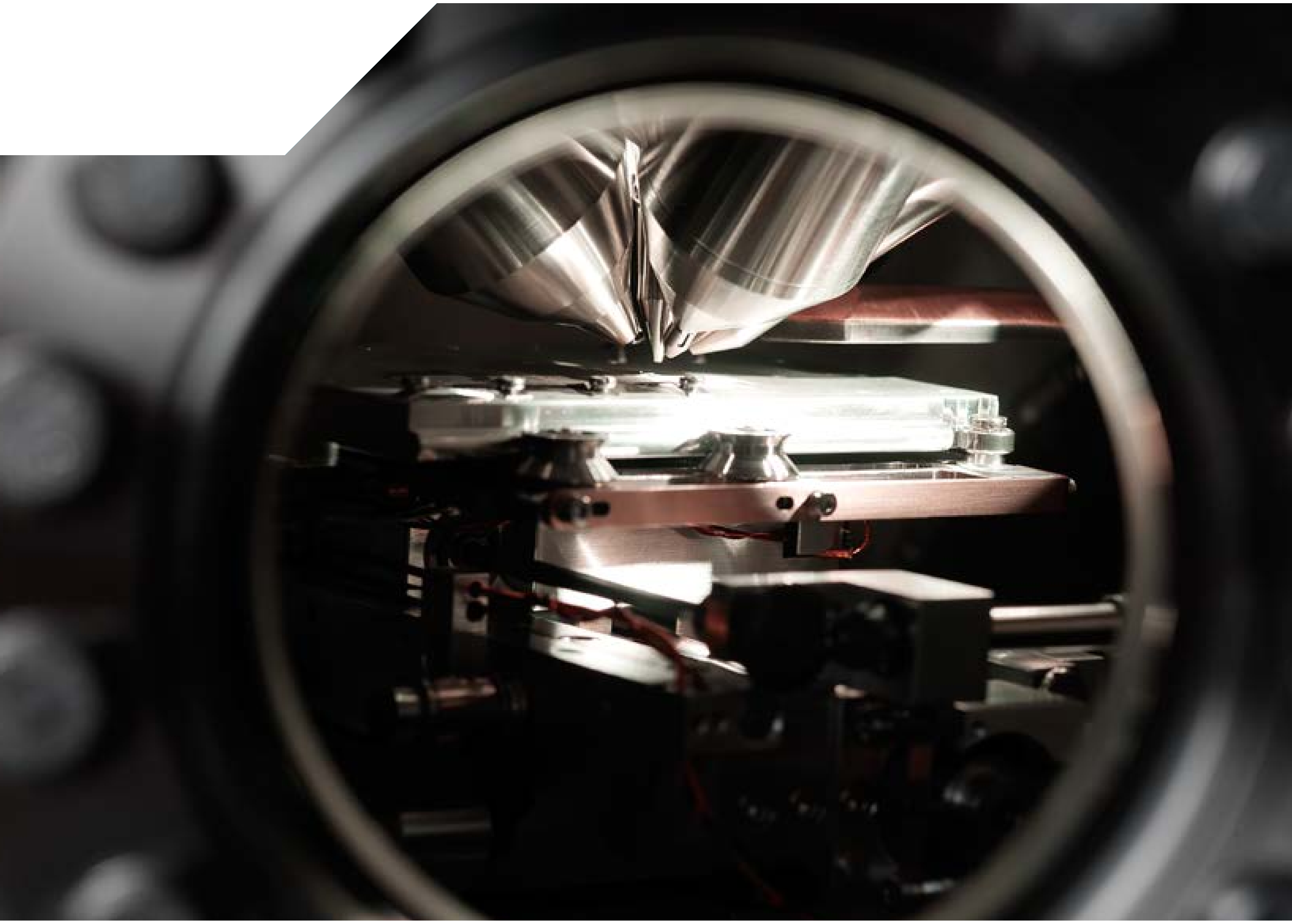
Scientific Innovation Through Integration

Investing in Innovation:

EMSL and the American Recovery and Reinvestment Act



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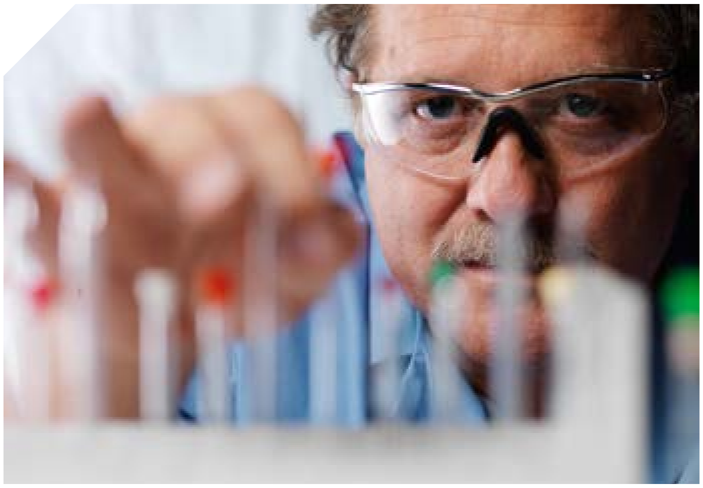
EMSL evolves with the needs of its scientific users, and the American Recovery and Reinvestment Act is helping to accelerate this evolution. On behalf of the Recovery Act, EMSL users are benefitting from a $60 million investment in innovation that will further develop and deploy transformational capabilities that deliver scientific discoveries in support of DOE's mission.

This investment will help EMSL:

- Establish leadership in *in situ* chemical imaging and procure ultrahigh-resolution microscopy tools
- Acquire next-generation mass spectrometry capabilities with unparalleled sensitivity and dynamic range
- Obtain nuclear magnetic resonance capabilities for high-field radiological and environmental/catalysis applications
- Advance its computational chemistry software, NWChem, toward extreme-scale computing
- Retain and grow a talented scientific workforce with established and specialized scientific expertise
- Promote a path toward a solid economic recovery.

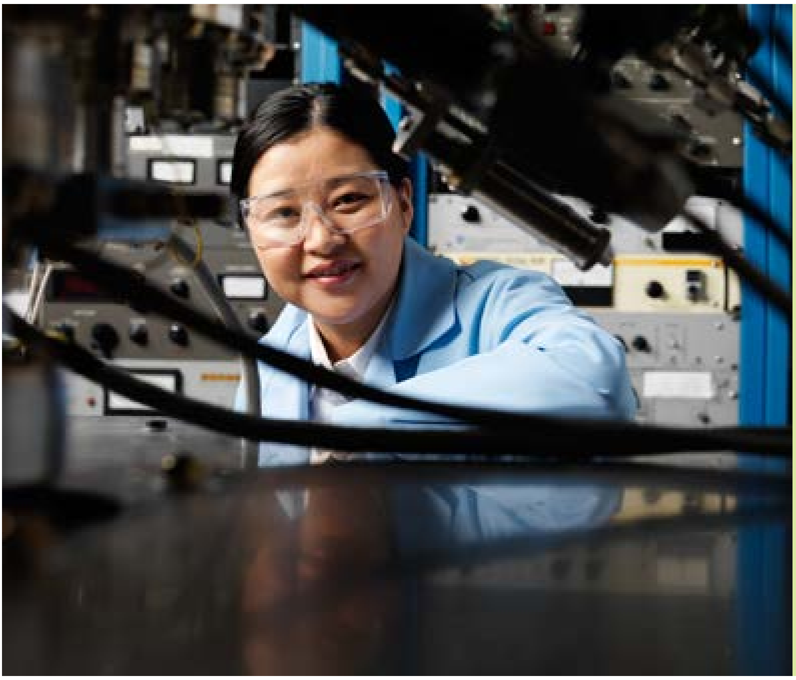
Each new and leading-edge EMSL instrument afforded by the Recovery Act was chosen by design to integrate well with one another as well as with the computational and experimental capabilities already housed in EMSL. Details about these instruments in the context of the existing EMSL capability group they support follow.



Cell Isolation and Systems Analysis

Multi-photon fluorescence microscope: Seamlessly integrates nonlinear two-photon excitation, laser scanning confocal microscopy and fluorescence lifetime imaging (FLIM) for minimally invasive and deep-penetrating 3D imaging of living tissues and cells as well as quantitative investigation of molecular interaction dynamics by fluorescence resonance energy transfer (FRET) in living cells.

Transcriptional profiling using next-generation sequencing technology (RNA-Seq): Offers massively parallel next-generation sequencing platforms for unbiased and quantitative profiling of gene expression patterns in prokaryotic and eukaryotic cells, complete with facilities for sample preparation as well as data processing and analysis.



Deposition and Microfabrication

Microfabrication capabilities: Deep reactive ion etching system can reproducibly fabricate high aspect-ratio microstructures with tight tolerances; offers multi-source sputter deposition system with *in situ* RHEED characterization along with e-beam sources and effusion cells for high-quality thin film growth, the ability to direct-write lithography to pattern features as small as 1 μm, as well as thermal and UV nano-imprinting capability for replication of patterns in the μm to nm range.

Mass Spectrometry

Advanced mass spectrometry capability: Orbitrap Velos ETD/H-ESI combines three different and complementary fragmentation techniques and represents the most comprehensive solution for analysis of post-translationally modified peptides and metabolites as well as for quantitative proteomics measurements.

Biomolecular imaging/mass microscope system: Combines C60 SIMS/MALDI-FTICR MS with an existing 9.4-Tesla magnet to effectively identify and characterize a diverse range of biomolecules. MALDI-TOF-based platform will offer 20-Hz acquisition speed and a resolution over 40,000 FWHM with sub-ppm mass measurement accuracy.

High-field Fourier transform ion cyclotron resonance mass spectrometry: 15-Tesla FT-ICR MS offers the highest mass resolving power and mass accuracy available on any commercial mass spectrometer, is a key technology for analyzing intact proteins (top-down mass spectrometry), and offers higher specificity for identifying metabolites and peptides from very complex mixtures (e.g., microbial communities) in a high-throughput fashion.

Ion mobility spectrometry-mass spectrometry proteomics system: Next-generation proteomics platform will combine liquid chromatography, IMS, and time-of-flight MS for increased throughput (10-50 times anticipated) and allow researchers to obtain systems biology information.

Isotopic mass spectrometry capability: Advances EMSL's elemental and isotopic analysis and characterization capabilities to include a multicollector plasma source MS as well as high- and ultra-high resolution plasma source MS to offer the ultimate performance in ratio precision, accuracy, and sensitivity.

Metallomics mass spectrometry capability: Combines ICP and ESI ionization with independent TOF-MS detection channels for the study of metals and their interactions and transformations in biological and environmental systems with the ability to acquire elemental and molecular chemical-state information simultaneously.

Next-generation metabolomics characterization capability: For global and targeted profiling of important metabolic pathways, fatty acids, and volatile molecules based on triple quadrupole MS coupled with GC or LC separations; the capability will be integrated with EMSL's existing 600-MHz LC-NMR platform, allowing multi-modal characterization of metabolite profiles and composition.

Microscopy

Environmental scanning electron microscope-focused ion beam system: Offers an enhanced ability to analyze wet and insulating materials; to analyze 3D section morphology, structure, and composition using FIB and electron backscattering diffraction/energy dispersive X-ray spectroscopy software; as well as to conduct high-temperature, gas interactions and selected area sample extraction studies.

Field-emission electron microprobe: A complement and enhancement to capabilities in electron microscopy, electron spectroscopy, and surface analysis, this new capability will be used to analyze solid-phase elemental concentrations at ppm levels using high-spatial resolution scanning electron microscopy with combined compositional information and cathodoluminescence imaging.

Geochemistry atomic force microscope: Offers atomic-scale imaging of mineral surfaces and local measurement of physical properties; advanced characterization of the electrical, magnetic, and surface potential properties of mineral surfaces; and is well suited for integration with EMSL's geochemical computation capabilities.

Helium ion microscope: One of only a handful of instruments in the world for cutting-edge imaging and chemical analysis with extremely high spatial resolution (0.35 nm), the He+ microscope offers the capability to image insulating specimens at high resolution without conductive coatings, provide image contrast for low Z elements, have large focus depth and high surface sensitivity as well as sharp Z contrast via backscattered ion imaging, and to conduct Rutherford backscattering analysis with a sub-nanometer He+ probe.

Infrared chemical nano-imaging and spectroscopy capability: The first environmental, tunable, infrared scattering-type scanning near-field microscope, this instrument uses infrared vibrational spectroscopy for molecular-specific imaging with 20-nanometer-scale spatial resolution.

Low-temperature scanning probe microscopy capability: A preeminent system for probing single-site chemical reactivity, this capability expands upon EMSL's existing capabilities for chemical imaging with atomic resolution, featuring true cryo (5K) scanning tunneling and non-contact atomic force microscopy, as well as the ability to combine *in situ* imaging with a hyperthermal molecular beam, single-molecule vibrational spectroscopy, as well as traditional ensemble-averaging surface analytical tools (XPS, UPS, AES, LEED, ISS).

Radiological scanning electron microscope/focused ion beam: Offers the ability to image and analyze radiological materials with high spatial resolution with 3D section analysis using FIB and electron backscattering diffraction/energy dispersive X-ray spectroscopy software and site-specific transmission electron microscopy sample preparation.

Scanning/transmission electron microscopy: Offers a combination of monochromatic and probe-corrected electron beam with a 1-Å STEM resolution and 0.3-eV energy resolution for single atomic column structure and chemical composition analysis, as well as simultaneous acquisition of chemical and structural information.

Subsurface Flow and Transport

X-ray computed tomography: Allows more accurate hydrologic models of the subsurface environment via acquisition of 3D images of pore space and connectivity of 10-cm diameter cores at 100-micron resolution, as well as provides the structural basis for interpretation of bulk property measurement such as hydrologic conductivity.

NMR and EPR

Catalysis/solids 850-MHz WB NMR system: The first of its kind in North America, the system will be dedicated to solid-state NMR and applicable to catalysis, energy, and bio-solids/surface interactions complete with *in situ* high-temperature and constant-flow probes, including a 60-kHz probe to allow the highest resolution of complex materials in the solid state.

Console upgrades for NMR systems: Upgrades EMSL to offer the latest generation in NMR consoles to support the most modern and demanding pulse sequences for users of 900-MHz, 800-MHz, 750-MHz, 500-MHz wide-bore imaging, and 300-MHz wide-bore NMR systems.

High-field EPR (95-GHz) system: One of only three systems of its kind with high-power capability worldwide, the system is designed not only for high field but high power (1 kW vs. 70-400 mW), sharply reducing acquisition time; the instrument will allow the study of integer spin metal centers like Ni(II) that are "EPR silent" at low field and easier interpretation of the spectra of high-spin systems (molecular magnets, e.g., Mn(II)).

***In situ* and bioreactivity NMR probes:** Novel probes designed and built by EMSL will include second-generation (multinuclear) bioreactor/biofilm (500-MHz wide-bore) and *in situ* catalysis probes to study higher field, low frequency nuclei, such as Mg, Zn, Ti, using the new 850-MHz wide-bore NMR; probes will allow for temperature extremes and include a novel cryo-magic angle spinning design for examining metallocenters in synthetic and natural contexts (500 MHz wide-bore).

Radiological/environmental 750-MHz WB NMR: The highest field radiological NMR in the world will allow solids, liquids, and imaging capabilities for the study of environmental and radiological samples as well as the ability to integrate experimental tools with NMR spectral simulation programs and *ab initio* techniques to derive magnetic resonance parameters from first principles structures. Multi-nuclear imaging/spectroscopy for observation of ^{1}H-^{13}C, ^{1}H -^{31}P and ^{1}H-^{99}Tc will enable spatial distribution/quantitation of ^{13}C, ^{31}P, and ^{99}Tc species in environmental/microbial sample systems.

Molecular Science Computing

NWChem new technology development cluster: Named "Barracuda," this cluster has leading-edge hardware technologies, such as GPGPUs, and advanced solid-state storage and networks that will enable crucial software advancements in NWChem to ensure readiness for HPCS-4 and to access new science utilizing extreme scale computing.

Archive storage capability: Named "Aurora," this 4.5 petabyte, energy efficient, and easily scalable scientific data archive will house the many terabytes of data generated per month by experimental and computational capabilities at EMSL.

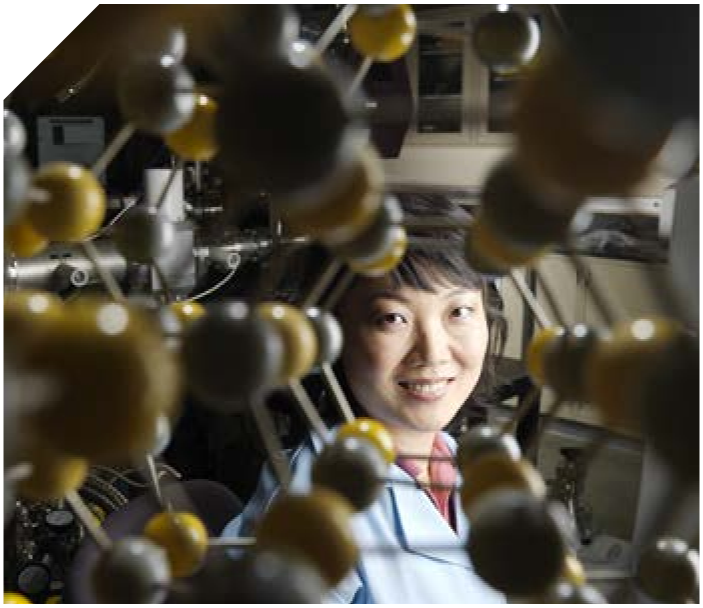
Spectroscopy and Diffraction

Accelerator upgrade, high-resolution RBS and triple beam facility: Offers high depth resolution RBS detector, a stable ion beam for high-resolution spectrometry and triple beam (ion, photon, and electron) radiation and characterization capability, as well as steady-state and time-resolved spectrofluorometer with 200 to 1900-nm wavelengths.

High-sensitivity X-ray photoelectron spectroscopy for radioactive materials: Dedicated high sensitivity XPS instrumentation equipped with mono-chromatic Ag Kα X-rays (for high Z elements), glove box for sample processing and transfer under a controlled environment, and cryo-cooling for wet materials; combines spectroscopy and imaging to provide actinide distribution on natural mineral and biological surfaces.

Laser-assisted atom probe tomography: Combined atomic-scale point-projection microscope and TOF MS is optimized for insulator analysis to yield information about grain boundary segregation and diffusion, materials degradation and failure, microstructural evolution, defect migration and cluster formation, nucleation and growth of materials with buried interfaces and related aspects through 3D chemical imaging with fraction-of-a-nanometer resolution and ppm sensitivity and affords the opportunity to integrate with EMSL's computational resources to efficiently reconstruct structure and composition.

X-ray photoelectron spectroscopy capability for chemical imaging: Combined with *in situ* temperature-programmed desorption and ultraviolet photoelectron spectroscopy, this instrument is unique in providing chemical, electronic structural, and morphological information before/after reactions and includes a side chamber equipped with a glove box for sample processing and transfer under a controlled environment, provisions to attach a reactor cell, and cryo-cooling for biological materials.



Become an EMSL User

Researchers from around the world are encouraged to submit a proposal to use EMSL's unique capabilities in combination with each other with an emphasis on merging computational and experimental instruments. To submit a proposal for use of EMSL or to learn more about the science conducted at EMSL and the instruments and expertise available to users, visit www.emsl.pnnl.gov.

Contact EMSL

Mark Bowden (*Spectroscopy & Diffraction, Subsurface Flow and Transport*)
Phone: 509-371-7816 | Email: mark.bowden@pnnl.gov

Nancy Washton (*NMR and EPR*)
Phone: 509-371-7094 | Email: nancy.washton@pnnl.gov

Galya Orr (*Cell Isolation and Systems Analysis*)
Phone: 509-371-6127 | Email: galya.orr@pnnl.gov

Ljiljana Paša-Tolić (*Mass Spectrometry*)
Phone: 509-371-6585 | Email: ljiljana.pasatolic@pnnl.gov

Theva Thevuthasan (*Deposition and Microfabrication*)
Phone: 509-371-6244 | Email: theva@pnnl.gov

David Cowley (*Molecular Science Computing, Operations*)
Phone: 509-371-6471 | Email: david.cowley@pnnl.gov

Bert de Jong (*Molecular Science Computing, Software*)
Phone: 509-371-6476 | Email: wibe.dejong@pnnl.gov

Erich Vorpagel (*Molecular Science Computing, Consulting*)
Phone: 509-371-6448 | Email: erich.vorpagel@pnnl.gov

Scott Lea (*Microscopy*)
Phone: 509-371-6233 | Email: scott.lea@pnnl.gov

User Support Office

Phone: 509-371-6003 | Email: emsl@pnnl.gov

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