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DOE

ENERGY SECRETARY HAZEL O'LEARY TO DEDICATE ENVIRONMENTAL MOLECULAR SCIENCES LABORATORY AT HANFORD

Energy Secretary Hazel R. O'Leary today dedicated the new Environmental Molecular Sciences Laboratory (EMSL) adjacent to the Department of Energy's (DOE) Hanford Site in north Richland, Washington. The laboratory will be operated by the DOE's Pacific Northwest National Laboratory (PNNL). EMSL will focus on developing the basic scientific understanding required by DOE to carry out its environmental restoration and waste management mission.

"Discoveries from this lab will provide the science needed to cleanup the nation's nuclear weapons production sites," said O'Leary. "Opening this laboratory reinforces President Clinton's strong belief that solving environmental problems leads to economic opportunity by creating new technologies, new businesses and new jobs."

At a ribbon cutting ceremony, the $230 million laboratory was named in honor of the late Dr. William R. Wiley, past PNNL Director, who championed basic molecular science research. Envisioned as a basic research center, Dr. Wiley and senior laboratory staff realized that science was poised to characterize, manipulate and create molecules to solve problems in environmental cleanup, energy efficiency, health and other fields. In April, 1994, Dr. Wiley said, "At Hanford and elsewhere, we have moved from the nuclear age to the molecular age."

The laboratory's 200,000 square feet will accommodate 270 staff with an annual operating budget between $60 and $70 million. EMSL will be home to some of the world's most sophisticated scientific equipment including the most powerful IBM parallel computer ever built. Additionally, the EMSL will receive the world's most powerful Nuclear Magnetic Resonance Spectrometer (NMRs) to be used in finding answers to biological and molecular problems related to human health and environmental restoration.

"The EMSL is a tangible, living testament to the Department's commitment to scientific research," said John Wagoner, Manager of the Department of Energy's Richland Operations Office. "It has a critical role in developing the technologies we need to get the job done in cleaning up Hanford safely and ahead of schedule."

At the dedication, Dr. Thom Dunning, EMSL Director, recalled his statement at the initial groundbreaking in July, 1994 when he said, "We are developing research capabilities that do not exist anywhere else in the world."

A unique aspect of the laboratory is its design as a Collaborative User Facility. In this role, EMSL will serve both the DOE mission and the external scientific community from universities, industry, and other federal laboratories. The `Collaboratory', as its known, will allow real-time remote interaction with remote instruments and software, and access to remote data and visualizations. It will also provide

education and training opportunities for the scientific and technical community.

"In the years ahead, scientists in EMSL will fulfill the destiny Bill Wiley envisioned for this laboratory by contributing solutions not only to environmental cleanup but also to domestic and global issues in energy, health, and national security," said Dr. Bill Madia, Director, Pacific Northwest National Laboratory.

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Overview -- Environmental Molecular Sciences Laboratory

The cost of cleaning up America's contaminated soils, and surface and ground waters using current technology is conservatively placed at more than one trillion dollars. Furthermore, technologies don't exist that can permanently and economically solve the most complex contamination problems.

The U.S. Department of Energy's Environmental Molecular Sciences Laboratory (EMSL) will develop the advanced science and technology necessary to clean up environmental problems at government and industrial sites across the country in an economically-viable manner. Research conducted at the national scientific user facility also is expected to lead to advances in energy, new materials, health and medicine, transportation and agriculture.

Construction of the EMSL is nearing completion at DOE's Pacific Northwest National Laboratory in Richland, Wash.

The 200,000-square-foot EMSL will house up to 270 staff, postdoctoral associates, visiting scientists and students. The research facility will cost $230 million and have an annual operating budget of between $60 million and $70 million.

An important component of the EMSL is its collaborative research environment. The Collaboratory, as it's often called, is a formal mechanism for EMSL researchers to share expertise, data, and the facilityþs unique scientific instruments with colleagues around the world. It also provides EMSL researchers with access to remote scientific information and capabilities that can be applied to their own environmental and molecular science research. More than 200 collaborative working agreements have been signed with university, government and private industry laboratories worldwide.

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History -- Environmental Molecular Sciences Laboratory

The concept of a research center dedicated to molecular sciences was introduced as a basic research initiative as part of the U.S. Department of Energy's Pacific Northwest National Laboratory's Institutional Plan process in 1986. Under the leadership of Dr. William R. Wiley, who was laboratory director at the time, Pacific Northwest committed to make a major investment of discretionary resources to address a scientific need identified by a National Academy of Sciences report titled "Opportunities in Chemistry."

Wiley and others at Pacific Northwest noted that recent advances in science and computers enabled scientists, for the first time, to characterize, manipulate and create molecules to solve problems associated with environmental cleanup, energy efficiency, health and other fields.

As envisioned at the time, the research center would bring theoreticians with expertise in computer modeling together with experimentalist in the physical and life sciences, and provide them with access to state-of-the-art research equipment and advanced computational and graphical capabilities. Research

would focus on the characterization of molecular structure, and the measurement and prediction of the properties and behavior of substances at the molecular and atomic levels.

During 1987, the laboratory formed a series of task forces representing the life, chemical, materials, earth and environmental, and computational sciences to develop plans for the center's major research programs and associated facility needs. An advisory panel of nationally prominent scientists drawn from universities, other national laboratories and industry was organized to participate in the planning phase.

By 1988, the center -- later named the Environmental Molecular Sciences Laboratory -- had evolved to be seen as a collaborative research facility to be available to the broader scientific community. In this setting, scientists and engineers from a wide variety of disciplines, such as physical, environmental, chemical, materials, biological, and computational sciences, would collaborate in basic experimental and theoretical molecular-level research focused on energy and environmental issues.

In 1989, Dr. Michael L. Knotek, former chairman of the Synchrotron Light Source at Brookhaven National Laboratory, was selected to lead the scientific planning for the EMSL and, simultaneously, to be Pacific Northwestþs senior science director. Dr. Steven D. Colson of Yale University became associate director for chemical structure and dynamics in June 1989, and two months later Dr. Thom H. Dunning, Jr., from Argonne National Laboratory, became associate director for theory, modeling, and simulation. With the arrival of these three distinguished individuals, the scientific foundation for the EMSL was in place.

In the spring of 1990, a panel was convened to conduct the EMSL's first major construction review. This panel concluded, "The intellectual challenge of the EMSL's mission is staggering. However, the practical payoff of success in this mission is immense, on the level of or perhaps beyond that of the Manhattan Project."

Over the next four years, the EMSL project was subjected to intense scrutiny and repeated reviews. The findings of these reviews consistently supported the EMSL research program and capability development activities that were undertaken by the staff and management of the EMSL and other organizations within Pacific Northwest.

Congress appropriated initial funding for EMSL design activities in 1989. In March 1994, Dunning was named EMSL director. Ground was broken in July that year, and construction on the $230 million international scientific user facility proceeded until its completion in fall 1996. Full-scale operations are scheduled to begin in 1997.

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Technology -- Environmental Molecular Sciences Laboratory

The U.S. Department of Energy's Environmental Molecular Sciences Laboratory (EMSL) will host some of the world's most sophisticated scientific equipment including:

IBM Supercomputer

The EMSL's 472-processor RS/6000 SP IBM supercomputer is the most powerful IBM parallel computer ever built and it will form the cornerstone of the EMSL's molecular science computing facility. Computational simulations and modeling performed on the supercomputer will further molecular-level understanding of the physical, chemical and biological processes that underlie environmental remediation, waste processing and related health and ecological effects.

Nuclear Magnetic Resonance Spectrometers

In early 1997, the EMSL will take delivery of the world's most powerful nuclear magnetic resonance spectrometer (NMRs), worth $10 million. NMRs are large, battery-shaped analytical tools that can provide molecular-level information about a variety of materials in their natural state, including inside the human body. They view microscopic objects by using superconducting magnets and radio waves. EMSL researchers will use the 900+ megahertz NMR as well as a suite of smaller NMR spectrometers to find answers to biological and molecular problems related to human health and environmental restoration.

Near-field Optical Microscope

A near-field optical microscope is a relatively new device which allows researchers to observe individual molecules in their natural biochemical environments at high resolution. The research has applications in several fields including chemical analysis, materials and the mapping of biological structures.

At the EMSL, the microscope is expected to have a major impact on the understanding of biochemical processes in biological membranes. The research may lead to advances in environmental cleanup science through a better understanding of how contaminants behave, migrate and diffuse at liquid-liquid and liquid-solid interactions. It also may lead to a better understanding of DNA damage, which in turn will lead to scientifically-based exposure standards for cleanup workers.

Powerful Mass Spectrometer

The EMSL will have the world's first 12-tesla mass spectrometer in a laboratory called the High Field Fourier Transform Ion Cyclotron Resonance Facility. Combined with special electrospray techniques, pioneered at Pacific Northwest National Laboratory, the powerful tool will examine biological molecules, including large molecules like DNA. The capability will allow researchers to study how the body's mechanism for repairing DNA, damaged by chemicals or radiation, sometimes goes awry. In addition, the instrument can help develop techniques to speed up the search for new prescription drugs.

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