# THE BIRTH OF A NATIONAL USER FACILITY

*EMSL–Molecular Science for the Environment*

10.16.1996

"WE HAVE MOVED FROM THE AGE OF ATOMS TO THE AGE OF MOLECULES."

WILLIAM R. WILEY

The genesis for the Environmental Molecular Sciences Laboratory can be traced to 1986. Laboratory Director William R. Wiley and a handful of his senior managers met to discuss how the Laboratory could respond to scientific challenges facing DOE, as identified in the National Academy of Sciences report entitled "Opportunities in Chemistry." This document, often referred to as the Pimentel Report, identified several scientific challenges relating to energy and the environment that depended on fundamental research in chemistry. The report went so far as to suggest that the missions of some of the national laboratories be reshaped to focus on these challenges.

The concept that came out of that meeting was for a center for molecular science research that would bring together theoreticians with expertise in computer modeling of molecular processes and experimentalists from the physical and life sciences. Wiley and others at the Laboratory, knowing of tremendous advances in scientists' abilities to characterize, manipulate, and create molecules, believed molecular-level research would be required to solve problems associated with environmental clean up, energy efficiency, health, and other fields.

Besides the NAS report, Wiley and his team had something else going for them. DOE, in cooperation with the White House's Office of Science and Technology Policy, believed each of its five multiprogram national Energy Research laboratories–Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge, and Pacific Northwest–should develop national scientific user facilities. While many of the other laboratories were envisioning large projects associated with high energy physics or synchrotron radiation, Wiley saw a need for a user facility dedicated to small science that would group together the most advanced equipment for molecular-level chemistry.

The 200,000-square-foot facility will contain experimental research programs in Chemical Structure and Dynamics; Materials and Interfaces; Macromolecular Structure and Dynamics; Theory, Modeling and Simulation; Environmental Dynamics and Simulation; Computing and Information Sciences; and Processing Science.

## MOVING ALONG

To start the process moving, Wiley assigned Ray Stults to develop a project team. Stults' first order of business was to write a proposal that demonstrated the scientific quality necessary to justify DOE's capital investment in such a facility and its equipment. Members of the proposal team were recruited from Battelle staff in Richland and in Columbus, Ohio; and during the height of the proposal activities, they numbered more than 50.

Adrian Roberts, currently director of the Economic Development Office at Pacific Northwest National Laboratory, became acting director of the Molecular Science Research Center, the initial name for the EMSL. Roberts commissioned production of a videotape and brochure, which were distributed extensively, as well as a series of progress reports, which were mailed to research universities and community and industry leaders. Then

Roberts began traveling throughout the Northwest region, creating presence and visibility for Wiley's vision as an investment in education and economic diversification for the region and the Tri-Cities.

IN NOVEMBER 1993, BILL WILEY AND MEMBERS OF THE EMSL TEAM CELEBRATE THE APPROVAL TO BEGIN CONSTRUCTION.

The Laboratory's operator, Ohio-based Battelle Memorial Institute, shared Wiley's enthusiasm for the project and gave the go-ahead to invest $8.5 million in discretionary resources in the EMSL over a 4-year period. With these funds, the Laboratory made plans for state-of-the-art research programs in molecular science and for bringing the equipment, facilities, and, most of all, people to support these programs.

It was a gamble. What scientist in his or her right mind would come to work on a nonexistent program, in a nonexistent facility, with nonexistent equipment, in Richland, Washington?

"If the scientific challenge is of such a nature to make it highly attractive, people will come," said Wiley at the time. "Nonexistent programs, facilities, and equipment can be sold to scientists of national and international repute, if they're driven by the nature of the challenge."

In 1988, Wiley hired Charles Duke, one of the nation's leading physicists and a senior research fellow with Xerox Corporation. Duke's 1-year contract called for him to develop the EMSL's initial research portfolio and to recruit critical scientific staff. Next, an advisory panel of prominent scientists from research universities, industry, and other national laboratories was organized to help shape the EMSL.

In 1989 Duke returned to Xerox and Michael L. Knotek, chairman of the National Synchrotron Light Source at Brookhaven National Laboratory, was hired to manage the EMSL project, along with Thom Dunning from Argonne National Laboratory and Steve Colson from Yale. Other leading scientists followed. Together they put the project on a much more aggressive scientific track. They believed the EMSL would need to define the leading edge in lab design, high-performance computing, and world-class instrumentation. They reconfigured the design to provide flexible lab space, free of vibrations and electrical interference. They also sharpened the environmental focus, adding programs in environmental dynamics and simulation and processing science, initially led by Rod Quinn.

Slowly, DOE and Congress saw the benefits of the proposed laboratory. Concerns that it was "pork" or a "make-work" project for unemployed DOE scientists gave way to a realization that the nation faced a daunting environmental problem, and the EMSL was a meritable scientific project able to contribute to the solution of several environmental restoration challenges.

DOE and Congress took note of peer reviews that supported the new laboratory and its likely contributions. "This research will increase our basic understanding of complex environmental systems leading to reduced costs, increased effectiveness, and decreased uncertainty in remedial actions," concluded a 1990 peer review report.

By 1993, the project had been scrutinized nearly 15 times by panels of science experts from government, research universities, and industry. Although the reviewers were tough, they consistently supported the need for the EMSL's capabilities. In addition, the Laboratory conducted nearly 20 technical workshops in which representative scientists were invited to help focus EMSL research on the most challenging problems.

Many people within DOE and Congress came to agree with the 1990 report, which 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."

## WHY AT PACIFIC NORTHWEST?

Once there was agreement on the need for this new capability, there also was strong agreement that a new facility had to be built. Available facilities at DOE sites were either decades old or too expensive to retrofit for the EMSL's advanced equipment and laboratories.

But where to build it? Some questioned whether PNNL—located in the sagebrush-covered Columbia Basin of eastern Washington State—was the best place. But many leaders saw PNNL's location as an asset. The national laboratory sits next to DOE's Hanford Site, which now stores the largest portion of the nation's toxic wastes generated over nearly 50 years of nuclear weapons production.

DOE also saw the EMSL as a natural extension of PNNL's mission. The national laboratory spends about one half of its $550 million annual budget on environmental research and development. With its location and environmental mission on its side, PNNL was authorized by DOE in October 1993 to proceed with construction, which began in July 1994 and is now complete. Installation of equipment will continue over the coming year and operations will formally begin in October 1997.

## THE RESEARCH HAS STARTED

PNNL and DOE aren't waiting for the new building to be finished before beginning work. Pending completion of the EMSL, dozens of research projects are under way in interim facilities. EMSL scientists are not conducting their research in a vacuum. They realize it takes a collaborative effort to develop permanent, safe, cost-effective solutions to the complex environmental problems our world is facing. As a result, more than 200 research collaborations with scientists at other national laboratories, research universities, and from industry have been set in motion.

"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."
*1990 Peer Review Report*

Although much of the initial EMSL research is driven by pressing environmental needs, research in the environmental molecular sciences will have far-ranging impacts in many areas. Research conducted at this national user facility is expected to lead to strategies for more efficient energy use, advanced processing technologies, innovative biomedical technologies, and advances in high-performance computing.

At least one project that doesn't concentrate only on environmental cleanup is already under way at the EMSL. Scientists have built and are using a near-field optical micro-

"THE PROBLEMS CAUSED BY TECHNOLOGY OVER THE LAST 50 YEARS WILL BE SOLVED BY TECHNOLOGY DEVELOPED AT THIS LABORATORY."

WILLIAM R. WILEY

scope for environmental research and also to learn more about how green plants capture the sun's energy and convert it to oxygen-producing flora. Understanding photosynthesis at the molecular level could lead to artificial photosynthetic systems to convert sunlight to chemical energy.

## TAKING A LEADING ROLE

The intellectual challenge presented by environmental stewardship is at least as great as that presented by the Manhattan Project in the 1940s and the space race in the 1960s and 1970s—and so is the potential payoff.

By understanding and controlling the molecular processes that underlie our environmental problems, DOE's William R. Wiley Environmental Molecular Sciences Laboratory will be a major contributor to solving some of the world's largest environmental problems.

### EMSL's Mission

The EMSL will serve as a national scientific user facility, focusing basic research on solving critical environmental problems. EMSL scientists will

- seek molecular-level understanding of the physical, chemical, and biological processes needed to solve environmental problems
- advance molecular science in support of long-term missions of the U.S. Department of Energy
- create a collaboratory, where unique research capabilities are made available to the broader scientific community using both traditional collaborations and the latest communications technology
- provide opportunities to educate and recruit the next generation of molecular scientists for tomorrow's challenges.

# WILLIAM R. WILEY ENVIRONMENTAL MOLECULAR SCIENCES LABORATORY DEDICATION

*October 16, 1996*

## PNNL Leadership

**Bill Madia,** Pacific Northwest National Laboratory Director • **Mike Knotek,** Director, Environmental and Energy Sciences Division • **Bill Shipp,** Director, Environmental Technology Division • **Ray Stults,** Program Manager, Environmental and Energy Sciences Division

## EMSL Leadership

**Thom Dunning, Jr.,** Director, EMSL • **Teresa Fryberger,** Deputy Director, Applied Environmental Science • **Shirley Rawson,** Acting Deputy Director, Environmental Remediation Science • **Steve Colson,** Associate Director, Chemical Structure and Dynamics • **Art Janata,** Associate Director, Materials and Interfaces • **Paul Ellis,** Associate Director, Macromolecular Structure and Dynamics • **Dave Dixon,** Associate Director, Theory, Modeling and Simulation • **Andy Felmy,** Acting Associate Director, Environmental Dynamics and Simulation • **Ray Bair**, Deputy Center Manager, Computing and Information Sciences • **Bruce Bunker,** Associate Director, Processing Science • **Dale Knutson,** Operations Manager • **Jim Bixler,** Manager, EMSL Construction Project • **Montcalm T. Thomas** (retired) and **James K. McCluskey,** Former Managers, EMSL Construction Project

## EMSL Advisory Committee

**Dr. Jerry Ebner (Chair),** Monsanto Company • **Dr. Sally Benson,** Lawrence Berkeley National Laboratory • **Dr. Richard A. Brouns,** Pacific Northwest National Laboratory • **Dr. Thomas Engel,** University of Washington • **Dr. James B. Harsh,** Washington State University • **Professor Steve Kevan,** University of Oregon • **Dr. Mel Koch,** University of Washington • **Professor Edward Lazowska,** University of Washington • **Dr. Bruce A. Moyer,** Oak Ridge National Laboratory • **Dr. Dhanpat Rai,** Pacific Northwest National Laboratory • **Dr. Leonard D. Spicer,** Duke University • **Dr. Peter R. Taylor,** San Diego Supercomputer Center • **Professor Robert O. Watts,** The University of Melbourne • **Dr. William J. Weber,** Pacific Northwest National Laboratory

## Speakers

**John Wagoner**
Manager, Richland Operations Office

**Bill Madia,** Director
Pacific Northwest National Laboratory

**Martha Krebs**
Director, Office of Energy Research

**The Honorable Norm Dicks**
U.S. House of Representatives

**The Honorable Richard (Doc) Hastings**
U.S. House of Representatives

**The Honorable Patty Murray**
U.S. Senate

**The Honorable Hazel O'Leary**
Secretary of Energy

**Mrs. William R. Wiley**

William R. Wiley EMSL
Environmental Molecular Sciences Laboratory