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Environmental Molecular Sciences Laboratory

William R. Wiley
EMSL NEWS
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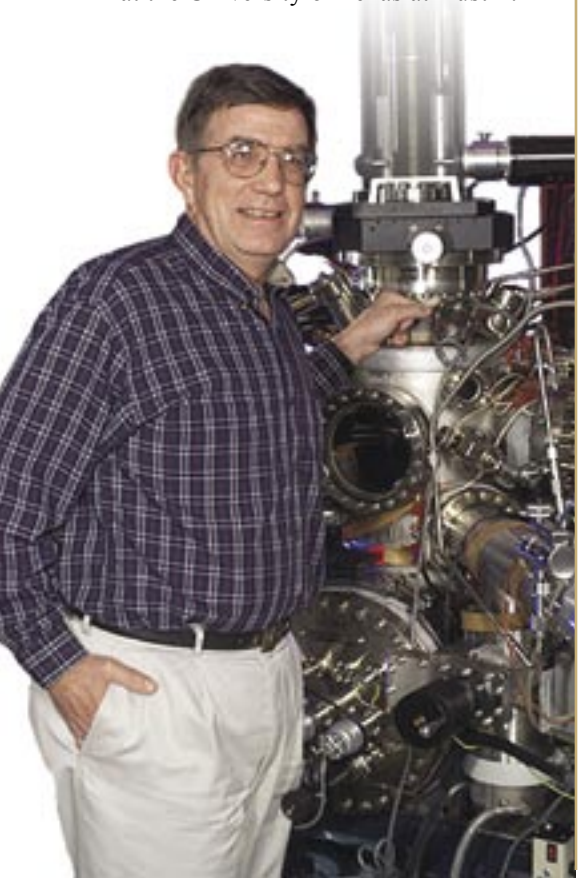
Renowned Surface Chemist Visits EMSL

Fundamental oxide surface chemistry to achieve self-cleaning glass

This summer, EMSL's Interfacial and Nanoscale Science Facility (INSF) hosted and continued collaborations with prestigious user J. Mike White, a Robert A. Welch Chair of Chemistry at the University of Texas at Austin.



As part of his visit—the second in two years—the prominent surface chemist analyzed data obtained during his first visit to EMSL in 2003. During that time, White used the EMSL's state-of-the-art equipment and laboratories to study self-cleaning glass—in particular, the fundamentals of photocatalytic reactions on titanium dioxide, a material usually found in house paint, and how the surface of the film is freed from "greasy-waxy" organic molecules that cause water beading.

In this fundamental study, the surface of a single crystal of titanium dioxide was adsorbed with an organic acid—similar to purified vinegar. Ultraviolet light is then "shined" on the sample, whereupon certain colors of the light spectrum activate the titanium dioxide, which in turn reacts with the adsorbed acid and generates carbon dioxide resulting in a clean sample surface. White and his collaborators used EMSL resources, such as electron energy loss spectroscopy and an ultrahigh vacuum chamber, to study these reactions.

"Self-cleaning is photo driven—light must be present," says White, who in 1989 received a plaque etched with the saying "Shine light on it" while being presented the Humboldt Senior Scientist Award from the Fritz-Haber Institute in Berlin.

This collaborative research has resulted in the "world's best hydrophobic surface that is one layer thick; easy to make and reproduce; and has interesting photo, electron, and thermal response."

"It has the potential to become a valuable prototype," says White, acknowledging that his goal is to understand the natural phenomenon and that the process of seeking a manufacturer is not his area of expertise.

(see ***Mike White***, page 4)

Mike White stands next to the Ultrahigh Vacuum Chamber, one of the critical pieces of equipment used during his research at EMSL. This chamber contains a titanium dioxide single crystal sample covered with one layer of molecules that undergoes light, temperature, and spectroscopic analysis to determine the properties needed for achieving self-cleaning glass.

Open Yet Secure Computing

At the Environmental and Molecular Sciences Laboratory (EMSL), staff and collaborative users from academia, industry, and other national laboratories—including many who visit from other countries—must freely access EMSL data and computational systems while conducting research both from within the facility and remotely. However, the need for EMSL to provide open access to data and systems could expose resources across the Pacific Northwest National Laboratory (PNNL)—on whose campus EMSL resides and with whom EMSL shares many systems—to security issues, such as hacking and viruses.

To encourage open access while protecting PNNL from computational vulnerabilities, EMSL and PNNL implemented the "EMSL Enclave"—a series of firewalls that "compartmentalize" the user facility's computer network from that of PNNL's and the open internet.

"With this enclave, we hope that EMSL will be allowed more flexibility in its security policies without impacting PNNL security," says Linda Connell, EMSL's Computer and Network Services (CaNS) Technical Group Leader. "By separating our network and data from PNNL's, we expect that any risk we accept will not expose PNNL's data to the same risks."

A hierarchy of access requirements was implemented to provide EMSL and PNNL networks with appropriate levels of security while protecting them from compromise. Thus, staff and users access PNNL's network "remotely" from their offices using the same methods they would from home. Many staff connect daily using Virtual Private Network software—which affords security by directing the user through a virtual "tunnel" into the network, and a SecurID one-time password, which provides user authentication.

The enclave provides the foundation for easier access to EMSL by creating the framework for differentiating EMSL's computer security requirements from PNNL's. The three-year effort involved intense concerted effort by staff from CaNS and PNNL's Information Resource Management System, and Safeguards and Security groups.

EMSL Software to be Deployed for First-Ever Educational Use

For the first time, EMSL's Extensible Computational Chemistry Environment—or Ecce—is formally being used in a classroom setting by an institution for educational purposes.

Matthew Asplund, Assistant Professor of Chemistry at Brigham Young University, has persuaded the faculty of BYU's Chemistry Department to forego their current chemistry software and implement Ecce—a problem-solving environment for computational chemistry—in their physical chemistry lab classes. About 100 chemistry and biochemistry majors are benefiting from the use of Ecce during the fall and winter semesters.

"We have a large supercomputer complex at BYU, and using Ecce lets us leverage those machines to allow students to perform higher-level calculations than with our previous software," says Asplund. "One of our goals is to have the students calculate a moderate-sized molecule with a bunch of basis sets to show that variational theory really does work."

Asplund also cites Ecce's user friendliness and no cost as drivers for incorporating Ecce into BYU's curriculum.

Ecce provides a sophisticated graphical user interface, scientific visualization tools, and the underlying data management framework that enable scientists to efficiently set up calculations and store, retrieve, and analyze data produced by computational chemistry studies. The software has been downloaded by more than 400 sites with multiple users at each site.

"Users of Ecce range from grade school children who 'build' molecules, to the graduate level where students are beginning to explore atomic-level bonding, to professors who have incorporated Ecce into their research programs to set up problems, visualize results, and store solutions," says PNNL Computational Scientist Gary Black, an original developer of Ecce.

One thing that makes Ecce unique from other software packages is its comprehensive capabilities that take users from the beginning stages of the problem-solving process through the analysis stages.

ECCE
EXTENSIBLE COMPUTATIONAL CHEMISTRY ENVIRONMENT

Respected Local Teacher Completes Fifth Summer Appointment

Jim Hendricks and Gordon Anderson, Acting EMSL Associate Director for Scientific, Computational and User Resources

This summer, EMSL's Instrument Development Laboratory (IDL) hosted Jim Hendricks, technology instructor at Southridge High School, along with his student, Nathan Perry. Their four-week appointment illustrates how EMSL continues to contribute to the multidisciplinary education of next-generation scientists.

This year marked Hendricks' fifth summer at the IDL. Such appointments provide him the opportunity to bring laboratory experience to his students during the school year.

Under IDL staff mentorship, Hendricks honed his schematic capturing skills—where schematics are developed using Computer Aided Design tools, then tested using drafting software and turned into circuit boards—so he in turn can mentor his students in that area. In addition, Hendricks—who assigns his students each year to build sumo robots for competition—used IDL resources to simplify a complex circuit board normally used in their construction to eliminate common mistakes made by the students.

Hendricks shares his appointment each summer with one to two students from Southridge's Engineering Technology Academy who will be mentored by IDL staff during the school year—this year, Perry. To prepare Perry, the duo developed an athletic wrestling tournament timing clock that provides wireless pages to the referee once a match is completed—versus "whacking" the referee with a towel to get his attention. Battelle's Intellectual Property Office, located at the Pacific Northwest National Laboratory, has offered to assist with patenting the clock on a pro bono basis as a school-wide project.

> ***"I like observing how the technicians and scientists interact to solve science problems, and learn what skills they look for when hiring staff."***
>
> – Jim Hendricks
> Southridge High School
> Engineering Technology Instructor

"What I gain working at the IDL cannot be measured," says Hendricks. "I like observing how the technicians and scientists interact to solve science problems, and learning what skills they look for when hiring staff. Through these observations, I can better train my students and share with them how you must be a good presenter, writer, and technical reader. That, to me, is really valuable."

Xin Yang Awarded M.T. Thomas Outstanding Postdoctoral Honor

Xin Yang was the 2003 recipient of the annual M.T. Thomas Award for Outstanding Postdoctoral Achievement that was presented on August 10. A postdoc of Lai-Sheng Wang, adjunct PNNL staff member, he was selected for his contributions to the development of electrospray-photoelectron spectroscopy techniques and for leading its use in new research directions, including the investigation of complex anion solvations in the gas phase and the electronic structure of the active site of Fe-S proteins. His innovative studies on environmentally related solvated anions such as sulfate and nitrate and dicarboxylate dianions, which serve as models for peptide chains, have been published in *Science*, the *Journal of the American Chemical Society* and the *Journal of Physical Chemistry.*

This award is named after retired PNNL researcher Dr. M. Tom Thomas, who was instrumental in efforts towards the design and construction of EMSL.

Pictured left to right: EMSL Interim Director Allison Campbell, M.T. Thomas Award recipient Xin Yang, Lai-Sheng Wang, and Tom Thomas

Mike White (continued from page 1)

Such research requires a wide variety of configurations and instruments in the EMSL laboratories to achieve the desired results. For example, different colors of the ultraviolet light spectrum and oxygen and non-oxygen environments were used to determine which worked best to spur the desired reaction, and mass, vibrational, and electronic spectroscopies were important elements to measuring mass and light properties of the titanium dioxide samples.

White and his collaborators published three papers during the past year describing the research in the *Journal of the American Chemical Society* and *Journal of Physical Chemistry*, with a fourth currently in press. Two to three additional papers are now in progress. In all, White has more than 650 published papers.

The second "leg" of White's visit this year involved a collaborative project among various national laboratories and universities. White and post-doctoral fellow Oleksander Bondarchuk also used EMSL's cutting-edge capabilities —in particular, scanning tunneling microscopy—to investigate the fundamentals of potential heterogeneous catalysis applications of mixed oxides by depositing tungsten trioxide on the titanium dioxide single crystals. Such applications include achieving hydrogen gas that results from water splitting on the titanium dioxide. The research is ongoing and is supported by DOE's Office of Basic Energy Sciences.

In the future, White—who counts former EMSL Director J.W. Rogers, Jr. and fellow collaborator and Pacific Northwest National Laboratory researcher Mike Henderson among his former PhD students—plans to again use EMSL capabilities.

"I've been interested in oxide surface chemistry for a long time," says White. "From my point of view, there are two places in the world where there is a critical mass of expertise in that arena: one is the Fritz-Haber Institute in Berlin, and the other is EMSL."

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EMSL User Services
W.R. Wiley Environmental Molecular Sciences Laboratory
Pacific Northwest National Laboratory
P.O. Box 999
MS K8-84
Richland, WA 99352

The William R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a Department of Energy national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. The EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research.

For additional details about the capabilities and research being performed at EMSL, please visit our web site at http://www.emsl.pnl.gov or call us at 509-376-2553.