

EMSL Monthly Report
March 2003

The W.R. Wiley Environmental Molecular Sciences Laboratory (EMSL) is a U.S. Department of Energy (DOE) national scientific user facility located at Pacific Northwest National Laboratory (PNNL) in Richland, Washington. EMSL is operated by PNNL for the DOE Office of Biological and Environmental Research. At one location, EMSL offers a comprehensive array of leading-edge resources in six research facilities.

Access to the capabilities and instrumentation in EMSL facilities is obtained on a peer-reviewed proposal basis. Users are participants on accepted proposals. Staff members work with users to expedite access to the facilities and scientific expertise. The Monthly Report documents research and activities of EMSL staff and users.

Research Highlights

First Proteomic Results from Three Strains of *Borrelia*

DG Camp,^(a) and X Yang^(b)

(a) Pacific Northwest National Laboratory

(b) State University of New York, Stony Brook

An initial proteomic survey comparing three *Borrelia* strains provided insights into a new field for analyzing Lyme disease. By studying the proteomics of *Borrelia*, protein targets are identified that can be used for vaccine development and diagnosis kits. A single global tryptic digest of *Borrelia* proteins from each strain was subjected to high-resolution, phase capillary liquid chromatography coupled with MS/MS analysis for peptide identification. The sequenced B31 database was used as the template to identify peptides from all three strains (B31, N40, and JD1).

This initial proteomic experiment showed variations in the proteins detected as well as differences among strains in the number of unique peptides identified. Strain N40 showed a high percentage of protein overlap (88%) with strain B31, but contained approximately four times less unique peptide identifications (Table 1). The N40 proteins detected most likely represent the most highly conserved proteins in comparison to B31. Strain JD1 showed a much lower protein overlap with B31 while containing the same number of protein

Table 1. Proteome variation in three different strains.

	Total peptides	Unique peptides	Peptide overlap with B31	Unique proteins	Protein overlap with B31
B31	1002	532	532/532 100%	116	116/116 100%
N40	166	128	98/128 77%	43	38/43 88%
JD1	953	587	239/587 41%	116	77/116 66%

identifications (Table 1). These results suggest a possible divergence of strains N40 and JD1 from B31 by two different methods. Strain N40 appears to show more sequence divergence from strain B31, while strain JD1 appears to display a different pattern of protein expression.

The subproteome analysis of each strain also proved insightful (Table 2). Three unique membrane proteins (BBA03, p66 and LMP1) are expressed in strain JD1 that are not detected in strain B31. The LMP1 protein has been shown to contain a unique amino acid repeated among different *Borrelia* species as well as in different human isolates. LMP1 may represent an important clinical marker for genomic studies, but further research is needed to substantiate this. Protein p66 has also been shown to have an important function in Lyme diagnosis. Unique heat shock proteins were also found in both JD1 and N40 strains that could assist in linking the function of proteins to differences in growth environments. These preliminary results demonstrate the possibilities of applying proteomic analyses of the *Borrelia* organism and related strains to further Lyme disease research.

Table 2. Proteins unique to strains N40 and JD1.

	Unique to strain	Hypothetical	Membrane	Heat shock	Ribosomal	Other function
N40	5	3/5 60%	1/5 20%	1/5 20%	X	X
JD1	39	15/39 38.5%	3/39 7.7%	3/39 7.7%	4/39 10%	14/39 36%

Adjustment of Perdew-Wang Exchange Functional for Describing van der Waals and DNA Base-Stacking Interactions

N Kurita,^(a) H Inoue,^(a) and H Sekino^(a)

(a) Toyohashi University of Technology, Toyohashi, Japan

Density functional theory calculations for van der Waals systems are an active area of research. Using NWChem software, Kurita and coworkers have examined modifications of the parameters for the Perdew-Wang (PW) functional to describe helium, neon, argon, and krypton dimers and DNA base-stacking interactions of cytosine monomers. This work, recently published in *Chemical Physics Letters*, shows that, with reparameterization of the d parameter in the PW functional, accurate binding energies can be obtained. However, it was also found that the appropriate value of d is largely dependent on the size of the atoms involved, with optimal values ranging from 3.3 to 4.1 for the dimers and 4.4 for the cytosine monomers. Clearly, additional investigations will be necessary to determine further terms needed to describe van der Waals interactions with the PW functional.

Transformation of Solid Atmospheric Particles into Liquid Droplets through Heterogeneous Chemistry

BJ Krueger,^(a) VH Grassian,^(a) A Laskin,^(b) and JP Cowin^(b)

(a) University of Iowa, Iowa City

(b) W.R. Wiley Environmental Molecular Sciences Laboratory

It has been reported that approximately 1000 to 3000 Tg of mineral aerosol are injected into the atmosphere as wind-blown soils annually. These particles have the potential to undergo a variety of heterogeneous reactions with atmospheric gases. In principle, it is possible that heterogeneous chemistry of atmospheric aerosol can change both the gas-phase chemical balance of the atmosphere and the physicochemical properties of individual particles. Changes in the properties of individual particles, such as size, shape, composition, and hygroscopicity, will alter aerosol optical properties and thus may have an impact on the Earth's climate.

To understand how individual particle properties affect reactivity, researchers Brenda Krueger and Vicki Grassian from the University of Iowa, working with EMSL staff members Alex Laskin and Jim Cowin, studied the real-time transformation of calcium carbonate particles. Calcium carbonate is a common component of mineral dust and may be a very reactive component of the aerosol present in the Earth's atmosphere. Using the Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray instruments located in EMSL, they examined the heterogeneous chemistry of individual calcium carbonate particles combining with nitric acid, a pervasive gas-phase species, to form calcium nitrate.

The data show that the reactivity of nitric acid is significantly enhanced in the presence of water vapor. The data also show that solid particles of calcium carbonate are transformed into aqueous calcium nitrate droplets as the particles react. The conversion of solid particles into liquid droplets through heterogeneous chemistry has important atmospheric implications in terms of the continued reactivity of the aerosol and the impact of the reacted aerosol on climate. As shown in these experiments (Figure 1), single-particle analysis can be used to determine changes in particle morphology, relative reaction rates, and the extent of reaction of individual particles as a function of particle size. A detailed report of this work appears in *Geophysical Research Letters* 30(3), 1148 (2003).

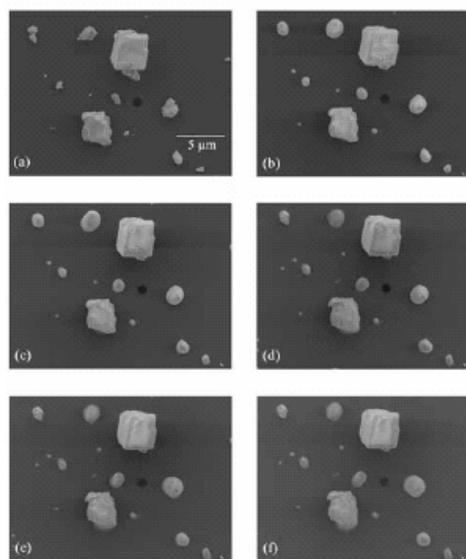


Figure 1. SEM images of calcium carbonate particles exposed to 20 mtorr of HNO_3 at $17 \pm 1\%$ RH: (a) before exposure, and after exposure for (b) 5 hours, (b) 10 hours, (c) 15 hours, (e) 20 hours, and (f) 26 hours.

Proximity Effects on Semiconducting Mineral Surfaces: Distance Dependence of Indirect Interactions

KM Rosso,^(a) and U Becker^(b)

(a) Pacific Northwest National Laboratory

(b) University of Michigan, Ann Arbor

In a previous study, we described proximity effects on surfaces of the semiconducting minerals galena and pyrite, whereby a chemical reaction at one surface site modifies the reactivity of a remote surface site several Angstroms or even nanometers away. The modification of interest does not arise because of a direct “through space” interaction between the two sites, but rather as an indirect interaction via the electronic structure of the substrate. Here we investigate the distance and direction dependence of proximity effects using quantum mechanical modeling. The direct and indirect interactions between co-adsorbed oxygen atoms and between adsorbed oxygen atoms and point defects on vacuum-terminated galena (100) surfaces were modeled. Density functional theory cluster and plane-wave pseudopotential calculations were used to calculate the modifications to the adsorption energy as a function of separation. Energy-distance plots (Figure 2) indicate that the proximity effect energy can become very strong at separations decreasing below about 5 to 6 Å, and persist at increasing

separations up to 12 Å in a slowly decaying form. A strong attractive indirect interaction out-competes direct electrostatic repulsion for O-vacancy interactions. An oscillatory asymptotic behavior is found for co-adsorbed O-O indirect interactions, which indicates that the proximity effect energy can vary with surface crystallographic direction. It implies the presence of a strong organizing force on like atoms that may explain the progressive oxidation of certain sulfide minerals by patchwork growth. These findings begin to pave the way for improved adsorption isotherms and extended surface complexation models that will include the specific influence of semiconductor-type proximity effects.

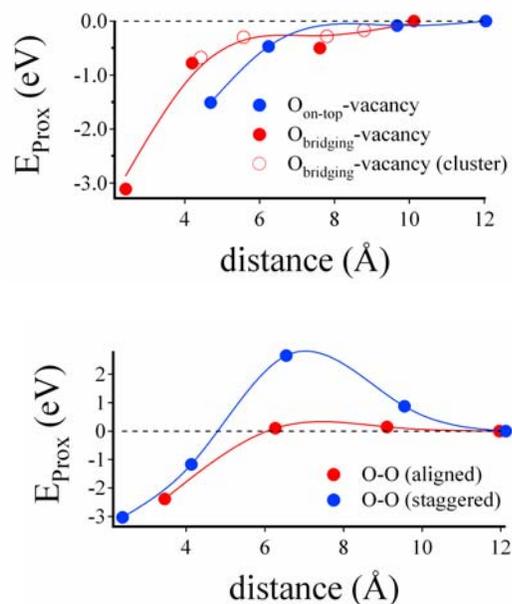


Figure 2. Energy-distance plots from the plane-wave pseudopotential method for the periodic slab treatment. Top graphic: The distance dependence of the indirect O-vacancy interactions, including the B3LYP cluster results. An attractive interaction dominates, increases in magnitude with decreasing distance, and decays slowly with increasing distance. Bottom graphic: The distance dependence of the indirect co-adsorbed O-O interactions showing an oscillatory attractive/repulsive behavior. The plots also show that the energy of indirect interaction is direction dependent. Cubic spline fits are shown to guide the eye.

NMR Analysis of Methyl Groups in Protein Model Systems up to 560 kDa

M Kreishman-Deitrick,^(a) C Egile,^(b) DW Hoyt,^(c) J Ford,^(c) R Li,^(b) and MK Rosen^(a)

(a) University of Texas Southwestern Medical Center at Dallas

(b) Harvard Medical School, Boston, Massachusetts

(c) W.R. Wiley Environmental Molecular Sciences Laboratory

Biomolecular solution nuclear magnetic resonance (NMR) is an extremely powerful tool with which to study the structure, conformational dynamics, and ligand interactions of macromolecules and assemblies. A significant obstacle facing NMR spectroscopy of large proteins (over 75 kDa) is the rapid deterioration of NMR signals due to fast transverse relaxation. While most of the work to date has focused on NMR signals from protein amide groups, sidechain methyl groups offer a useful alternative spectroscopic probe in large systems.

Our time at EMSL has allowed us to establish the feasibility and scope of using methyl groups in NMR spectroscopy in molecules as large as 560 kDa. To establish the general utility of methyl groups in large systems, we used a test sample consisting of a 16 kDa protein suspended in a solution of 40% v/v glycerol. By exploiting the steep temperature dependence of glycerol solution viscosity, we were able to simulate a range of rotational correlation times (60 to 330 nanoseconds), which corresponds to a molecular weight range of about 100 to 560 kDa. The use of the high-field spectrometers available at EMSL allowed us to do a systematic, thorough analysis of $^1\text{H}/^{13}\text{C}$ -HSQC spectra of this protein at a variety of temperatures and at two different fields (Figure 3).

With the work performed at EMSL, we have established sidechain methyl groups as extremely sensitive probes for NMR spectroscopy of large molecules.

This work, "NMR Analysis of Methyl Groups in the 240 kDa Arp2/3 Complex and Model Systems up to 560 kDa" has been submitted to *Biochemistry*.

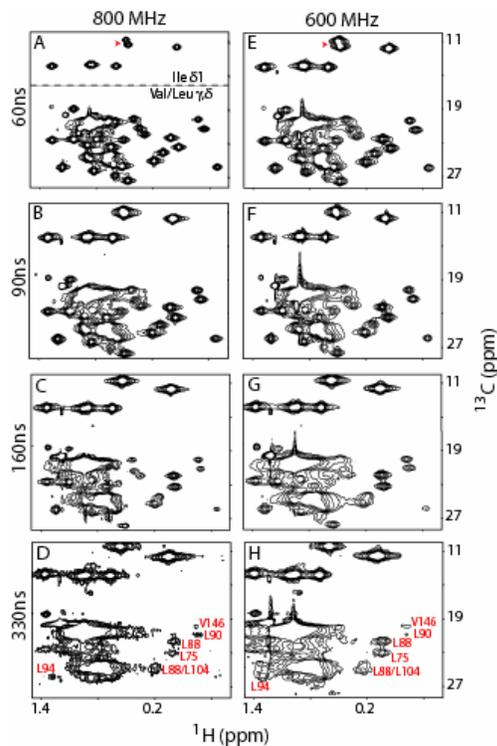


Figure 3. $^1\text{H}/^{13}\text{C}$ -HSQC spectra of a 16 kDa protein in 40% v/v glycerol. Spectra were acquired at the fields indicated, and at the following temperatures: 25°C (panels A and E), 15°C (B and F), 0°C (C and G) and -10°C (D and H). Estimated τ_c values for each temperature are shown to the left of each row.

Heteroepitaxial Growth of a Manganese Carbonate Secondary Nano-phase on the $(1\ 0\ \bar{1}\ 4)$ Surface of Calcite in Solution

AS Lea,^(a) TT Hurt,^(b) A El-Azab,^(a) JE Amonette,^(a) and DR Baer^(a)

(a) Pacific Northwest National Laboratory

(b) Cornell University, Ithaca, New York

Heteroepitaxy of a manganese carbonate phase with nanometer dimensions on the $(1\ 0\ \bar{1}\ 4)$ surface of calcite (CaCO_3) using an Atomic Force Microscope (AFM) has been observed in solution during dissolution of calcite when the ion activity product of Mn^{2+} and CO_3^{2-} nears the solubility limit of MnCO_3 (Figure 4). Growth rate observations at different manganese concentrations, coupled with X-ray photoelectron spectroscopy and electron paramagnetic resonance measurements, suggest that the resulting phase is $\text{Mn}_{0.5}\text{Ca}_{0.5}\text{CO}_3$. These islands, while growing many microns in length along the $[2\ \bar{2}\ 1]$ direction, have a uniform width in the range of 120 to 240 nanometers and a uniform height of approximately 2.7 nanometers, corresponding to nine atomic layers. The islands cease growing when they encounter step edges and have been observed to dissolve when undercut by a growing etch pit.

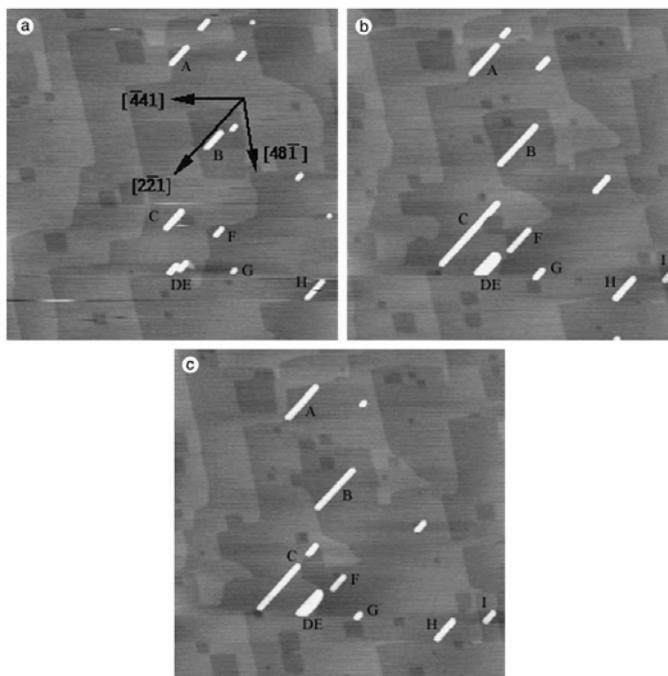


Figure 4. 1.7.0 μm AFM topographic images of the $(1\ 0\ \bar{1}\ 4)$ surface of calcite in a pH 8.9 150 μM carbonate solution containing 2 μM Mn^{2+} . Visible in the images are 3.14 \AA single steps, single- and multilayer deep etch pits, and highly oriented precipitates on the surface of calcite. (b) and (c) are images taken 11 and 26 minutes after the first image (a). Superimposed on the image in (a) are the principle crystallographic axes on the calcite surface.

Comparison of the crystal lattices of calcite and $\text{Mn}_{0.5}\text{Ca}_{0.5}\text{CO}_3$ indicates that $[2\ \bar{2}\ 1]$ is the direction of preferred growth. A glued-wetting-layer model with a condition of constant surface chemical potential has been used to model the observed cross section of the heteroepitaxial layer. Although not all the required parameters are accurately known, the model accurately depicts the measured profiles of the islands.

Proton Transfer Reaction Ion Trap Mass Spectrometry

M Alexander,^(a) P Prazeller,^(a) BT Jobson,^(a) and P Palmer^(b)

(a) Pacific Northwest National Laboratory

(b) San Francisco State University, San Francisco, California

Proton Transfer Reaction Mass Spectrometry (PTR-MS) is a relatively new field that has attracted a great deal of interest in the last several years. This technique uses H_3O^+ as a chemical ionization agent. The advantages of PTR-MS include high sensitivity, selectivity, and accuracy. A commercial PTR-MS was purchased in Fiscal Year 2001. The PTR-MS mass spectra are simpler than those obtained by conventional electron-impact spectra because the ionization method—transfer of a proton—is “soft” resulting in little fragmentation. This can cause problems in peak identification, however, due to isobaric interferences. A possible solution to this problem is to couple the PTR drift tube to an ion trap mass spectrometer (ITMS). This has been the subject of much speculation and discussion in the PTR-MS community. ITMS is appealing because of the ability to perform MS-MS and possibly distinguish between isomers and other isobars. It is also appealing because the duty cycle is much higher than a linear quadrupole so faster response time can be obtained for the detection of multiple compounds. This project represents the first successful effort in creating a PTR-ITMS (Figure 5).

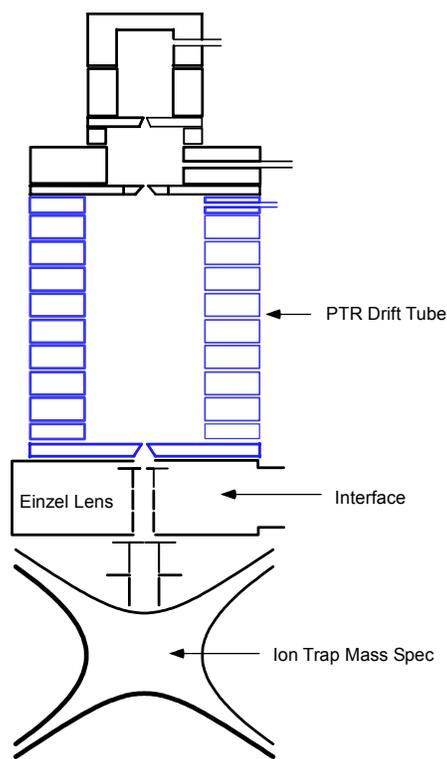


Figure 5. Schematic of PTR-ITMS showing drift tube, interface, and ITMS.

The first step was to run the trap at high pressure to compensate for the high ion energies required to make it through the interface. This resulted in a background level at least a factor of 100 higher than is normal for this detector. Simply implementing differential pumping can improve the sensitivity by this factor of 100. Better pumping in the interface can improve the signal by a factor of 10 to 100. This means that sensitivities of 1 parts per billion (ppb) should be possible. The other question that was addressed in this collaboration was how effective MS-MS in an ion trap will be in distinguishing isobars. One example is acetone and propanal, both of which have a protonated mass of 59. Figures 6a and 6b show that both compounds fragment into mass 41 and mass 31, but with different fragmentation ratios. These data indicate that MS-MS in the ITMS could distinguish between pure compounds, but mixtures would be hard to resolve. Figures 6c and 6d show similar data for methacrolein and methyl vinyl ketone (MVK), both of which have a protonated mass of 71. Methacrolein has fragments at 41 and 43 while MVK only produces a fragment at 43. We also note that the 43/41 branching ratio in methacrolein displays a dependence on the collision area, indicating some possibly interesting dynamics.

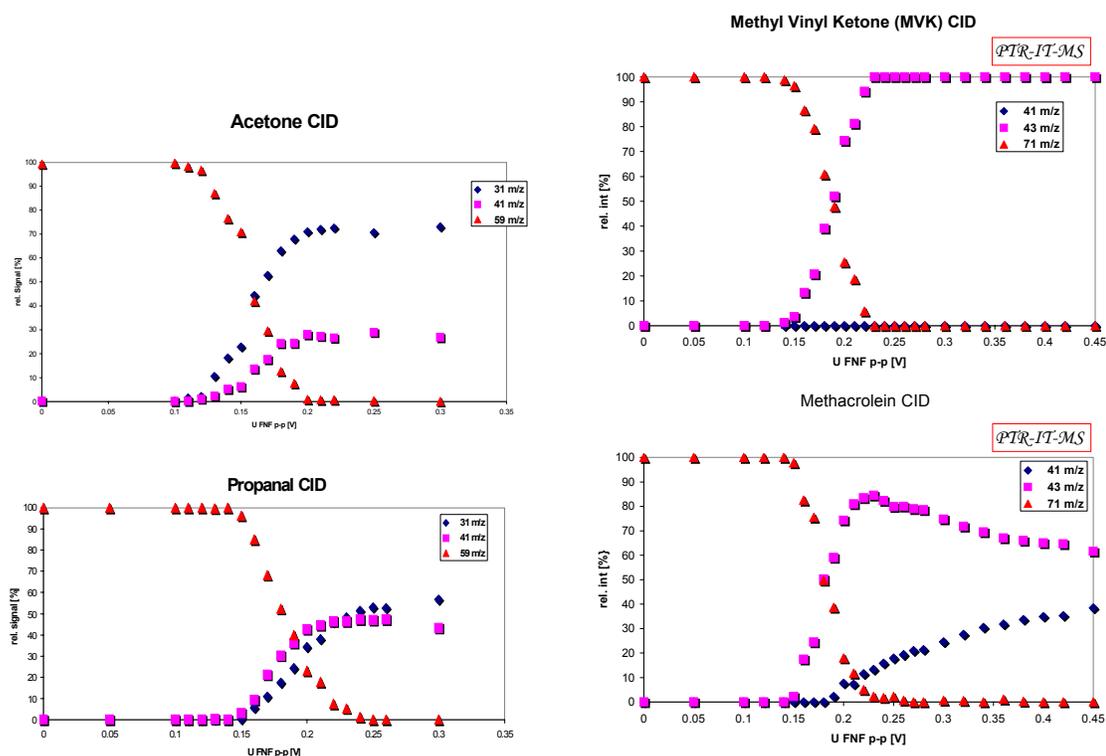


Figure 6. MS-MS spectra of protonated (a) acetone, (b) propanal, (c) MVK, and (d) methacrolein as a function of excitation voltage .

The data to date show a great deal of promise for PTR-ITMS. The sensitivity should ultimately be 1 ppb or better which, combined with the higher duty cycle inherent in ITMS, will make the PTR-ITMS a valuable tool for time-dependent studies. MS-MS can be a valuable tool for distinguishing between some isobars of protonated species. A second-generation instrument is currently being developed with results expected in mid-2003.

Awards and Recognition

John Zachara's presentation was selected as the most outstanding contribution from a national laboratory at the DOE Office of Basic Energy Science Geosciences Symposium on "Surficial Geochemical Processes," March 8, 2003. Authors of the work presented are John M. Zachara, Jim K. Fredrickson, Ravi K. Kukkadapu, and Chongxuan Liu.

Professional/Community Service

Udo Becker and Kevin Rosso organized and edited a special issue of *Geochimica et Cosmochimica Acta*, 67(5), (March 2003) consisting of 24 articles, focusing on mineral surfaces, that summarized the symposium, "Advances in Oxide and Sulfide Mineral Surface Geochemistry," held at the 2001 Goldschmidt meeting in Hot Springs, Virginia.

Nancy Foster-Mills is project director for Team Battelle Destination Imagination, a team-based creative problem solving program for children. She recruited judges and organized the Washington State Mid-Columbia Regional competition held in Richland, Washington on March 8, 2003.

Anna Cavinato of Eastern Oregon University, La Grande, and four undergraduate students (Richard Champion, Bina Hall, Dean Kuenzi, and Alicia McRoberts) recently visited for a one day hands-on class to learn how to assign chemical shifts of several dipeptides using 1-D and 2-D nuclear magnetic resonance (NMR) methods on a 500 MHz NMR system in the High-Field Magnetic Resonance Facility (Figure 7). This lab was taught by EMSL scientists David Hoyt and Joseph Ford. The students learned basic spectrometer operation skills and were given a perspective of how NMR is used to determine critical structural information of larger biomolecules. Additional instruction was given by PNNL postdoctoral fellow John Bagu and a visiting EMSL user Peter Brzovic (University of Washington, Seattle). A graphics presentation was also given by EMSL scientist Erich Vorpapel of the Molecular Science Computing Facility.



Figure 7. Students from Eastern Oregon University visit for a one-day class in the High-Field Magnetic Resonance Facility.

Major Facility Upgrades

Phase2 of the Hewlett-Packard (HP) supercomputer reached a major developmental milestone in March by sustaining greater than 4.8 teraflops on the linpack benchmark. This would have placed the system as the sixth most powerful supercomputer in the world on last November's Top500 list (www.top500.org). The system is targeted to become operational by the end of the fiscal year, with early science runs commencing in June 2003.

The Molecular Science Computing Facility (MSCF) operations group collaborated with HP on the “smart cooling” design for the MSCF. The smart cooling design is targeted toward providing the appropriate level of cooling for the computer room rather than over-engineering the cooling. The final design is projected to save EMSL a large fraction of the electrical bill for cooling the 750 KVA computer room.

In March, MSCF staff came one step closer to reaching stability with the Lustre filesystem. They were able to sustain a write rate of greater than 2GB per second to a 50 terabyte filesystem. This is two orders of magnitude faster than the previous global filesystem that was used on the IBM SP.

A beta version of NWChem 4.5 is now available for users to download and test. Major additions to this version include the port to the Phase I system (Itanium 2 with Quadrics interconnect), a time-dependent density functional module that also includes configuration-interaction singles capability, an electron transfer module, a projected augmented wave module, and a tensor contraction engine module, which includes many high-level correlation methods created by an automated code generation package. Many other additions and bug fixes are also included in the 4.5 beta release. Initial feedback from users has been positive and all reported problems are being resolved.

News Coverage

An image created with resources in the MSCF Graphics and Visualization Lab was featured on the cover of *Resource Engineering and Technology for a Sustainable World*, 10(3) (March 2003). Advanced scientific research practices and equipment facilitate recovery of higher-value materials from agricultural byproduct streams. Spearheading development of an integrated process for such recovery, the cover story's research team employed highly sophisticated instrumentation, including a nuclear magnetic resonator, to disassemble corn fibers while ensuring the integrity of valuable trace fractions. (Figure 8 graphic art by Mike Perkins, James Franz, and Erich Vorpagel).

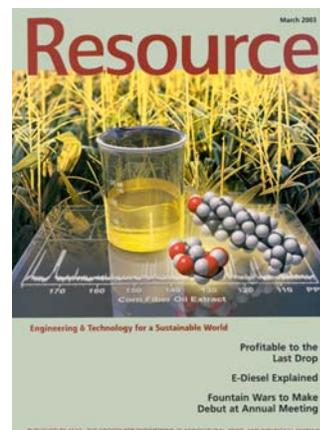


Figure 8. Image created at the MSCF.

An image created with resources in the MSCF Graphics and Visualization Lab was featured in the DOE Science News http://www.sc.doe.gov/Science_News/feature_articles_2003/January/enzyme/enzyme.htm. (Figure 9 graphic art by Mike Perkins). This is an artist's conception of a cutaway view of an immobilized enzyme within a functionalized nanoporous silica pore. The enzyme is shown as green with positively charged regions shown in red. The blue structures inside the pores represent the negatively charged functional groups added to the mesoporous silica to create a favorable chemical environment for the enzyme. The favorable environment in each pore attracts the enzyme molecule to move into the unoccupied pore. This environment stabilizes and increases the chemical reactivity of the enzyme, allowing it to convert harmful substrate materials (purple particles) into useful or harmless products (yellow and red particles).

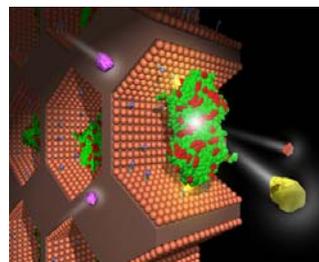


Figure 9. Enzyme within a functionalized nanoporous silica pore .

Spectroscopy Europe used on the cover of its March 2003 issue a photo of the 900-MHz nuclear NMR being lowered into EMSL. (<http://www.spectroscopyeurope.com/>).

Paul Ellis was quoted in a recent *Nature* article by Kendall Powell, "The data busters" (*Nature*, 421(6926) 970-973) about the importance of collaborative effort and use of high-field NMR spectrometers in structural genomics research.

David Bryce, University of Alberta/Dalhousie University in Halifax Nova Scotia, was featured in a news release that described his research at EMSL, where he used NMR spectroscopy to characterize three-dimensional interactions in elements such as boron, chlorine, and chromium. (http://www.nserc.ca/news/2003/p030328_b1.htm).

HPCwire, The Electronic News Magazine for Supercomputing, presents the news brief, "Platform Computing Software Powers PNNL Supercomputer", in the March 7, 2003: Vol. 12, No. 9 issue. (<http://www.tgc.com/hpc-bin/engine.pl?name=/articles/toc030703.html>).

Visitors and Users

Chemistry & Physics of Complex Systems

- Krishnamoorthy Kuppannan and Kristin Herrmann, University of Arizona, Tucson, worked with Julia Laskin to study how to implement Surface-Induced Dissociation (SID) into FT-MS. The research involves low-energy collisions of ions with well-ordered surfaces such as self-assembled monolayers (SAMs) of alkanethiols on gold or Langmuir-Blodgett (LB) films. The process of fragmentation (surface-induced dissociation) is the major experimental variable that is used in determination of peptide dissociation mechanisms for potential use in high throughput identification of proteins.

Environmental Spectroscopy & Biogeochemistry Facility

- Zbigniew Dreger, Washington State University, Pullman, visited EMSL to perform lifetime measurements of single crystal anthracene at elevated pressures following excitation into both the singlet and triplet excited states. Using EMSL's time-correlated single photon counting system and time-resolved nanosecond OPO laser system, Dr. Dreger expects to use these measurements to understand the role of nonhydrostatic stresses in the formation and modification of structural defects in these crystals.
- Daniela Bocioaga, University of Montana, Butte, visited EMSL to study distribution of trace metals on unicellular algae and bacteria in Berkeley Pit lake water. She used a high-resolution transmission electron microscope coupled with energy dispersive spectroscopy to visualize and analyze reduction products for evaluation of the sorption potential of these organisms and their bioremediation potential. The extent of metal uptake by algae was determined via inductively coupled plasma - mass spectrometry and atomic absorption.



Figure 10. Zbigniew Dreger (above) and Daniela Bocioaga.

High Field Magnetic Resonance Facility

- Kathryn Ely, The Burnum Institute, La Jolla, California, and postdoc Klara Briknarova used the 750-MHz spectrometer to work on the studies of “Structural Characterization of Free and Fibronectin-bound Anastellin.”
- John Hanna, Lucas Heights Research Laboratories, Australia, used the 500-MHz spectrometer for his studies of “Solid-State NMR Characterization of Metal Phosphines.”
- Evan R Kantrowitz, Boston College, used the 500-MHz spectrometer to work on the studies of “Probing the Mechanism of the Alkaline Phosphatase Reaction by ^{67}Zn and ^{25}Mg NMR.”
- Rachel E. Klevit, University of Washington, Seattle, sent Peter Brzovic, University of Washington Cell Systems Initiative, to EMSL to use both 600-MHz spectrometers for their project “NMR Structural Investigations of BRCA1.”
- David Kramer, Washington State University, Pullman, and graduate student Arthur G. Roberts came to use the FTEPR1 spectrometer to work on the studies of “Molecular Probes of Quinol Oxidation by the Cytochrome *b₆f* Complex.”
- Sarah C Larsen, University of Iowa, Iowa City, and graduate student James Francis Woodworth came to use the FTEPR1 spectrometer for work on “Pulsed EPR Studies of Transition Metal-Exchanged Zeolites and Molecular Sieves.”
- Michael K. Rosen and graduate student Mara Kreishman-Deitrick, University of Texas Southwestern Medical Center, Dallas, Texas, recently worked remotely on the 800-MHz spectrometer for their study of “Activation of the Arp2/3 Complex by WASP Family Proteins: Probing Individual Subunits by NMR.”

- Louis Silks, Los Alamos National Laboratory, Los Alamos, New Mexico, recently used the 500-MHz spectrometer to work on the studies of “Ultra-High Field NMR Studies of Stable Isotope Applications.”
- Gabriele Varani, University of Washington, Seattle, and graduate student Thomas Leeper recently used the 800-MHz spectrometer to work on the studies of “Structure of Human Telomerase RNA.”
- L. Q. Wang, Pacific Northwest National Laboratory, recently used the 500-MHz spectrometer to work on the studies of “Probing Nanostructural Materials.”

High Performance Mass Spectrometry Facility

- Michael Daly, Uniformed Services University of Health Sciences, Bethesda, Maryland, provided samples to the HPMSF for work on “Comparative Display of *D. radiodurans* after Exposure to Ionizing Radiation.”
- Ronald W. Davis and Wenzhong Xiao, Stanford University, Stanford, California, and Curt M Scharfe, Stanford University, Palo Alto, California, sent samples to the HPMSF for their work on “Functional Genomics and Proteomics of Mitochondria.”
- Xiaohua Yang, State University of New York, Stony Brook, provided cell samples of three different *Borrelia* strains for proteomic research on “Lyme Disease Spirochete Causative Agent.”
- Amy K Schmid, University of Washington, Seattle, performed research on her project “Identification of Heat Shock Proteins in the Radioresistant Bacterium *Deinococcus radiodurans*.”

Interfacial & Nanoscale Science Facility

- John Cliff, Oregon State University, Corvallis, used time-of-flight secondary ion mass spectrometry instrumentation to study the use of stable C and N isotopes to trace soil chemical processes and biogeochemical nutrient cycling in soils.
- Michael Donely, Wright-Patterson Air Force Base, Ohio, used time-of-flight secondary ion mass spectrometry instrumentation to study epoxy-zirconate sol-gel-based surface treatments.

Molecular Science Computing Facility

- Peter Braam, Cluster File Systems, Canmore, Alberta, Canada, visited to collaborate on the file design for the next-generation archive.
 - Anna G. Cavinato, Eastern Oregon University, La Grande, visited EMSL with eight students for a one-day demonstration of how NMR can be applied to solving protein structure and interactions. The Graphics and Visualization Lab was used to display and discuss the results using three-dimensional projection.
 - Natalia Tilkunova, Alexander Stepanov, and Dmitry Zalepugin visited from the State Research Institute of Organic Chemistry and Technology in Moscow, Russian Federation. They are partnering with PNNL on a project based on the synthesis of analogs of garlic extracts for development of new fluorinated anticancer compounds. They indicated that their areas of particular interest are in computational chemistry and supercritical fluids for extraction.
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- Four visitors from the PNNL's National Security Directorate toured the Graphics and Visualization Lab. The visitors, special programs clients, wanted to see the supercomputer and the VizLab/Collabrusuite technologies.
- EMSL Director Bill Rogers hosted five visitors from the Center for Integrated Nanotechnology, a joint user facility with Sandia and Los Alamos national laboratories. The visitors were interested in learning about EMSL as a user facility. The Graphics and Visualization Lab was one of their stops during their visit.

Molecular Sciences Software - New user agreements with NWChem/Ecce:

- Vibhas Aravamuthan, Louisiana State University, Baton Rouge, Louisiana
- Daryl G. Clerc, ArTek Product Development, Inc., Dexter, Michigan
- Roy Dragseth, University of Tromso, Tromso, Norway
- Nikolaus Heinrich, Schering Aktiengesellschaft, Berlin, Germany
- Victor Mashayekhi, Dell Computers, Round Rock, Texas
- Patrick Norman, Linkoping University, Linkoping, Sweden
- Glenisson de Oliveris, Rhode Island College, Providence, Rhode Island
- Ted Packwood, Cray Inc., Mendota Height, Minnesota
- Matt Reilly, SiCortex, Inc, Newton, Massachusetts
- Javier Sanz, University of Sevilla, Sevilla, Spain
- Masnanori Tachiya, Agency of Industrial Science and Technology, Ibaraki, Japan
- Fu-Ming Tao, California State University, Fullerton, California
- A. S. Trew, University of Edinburgh, Edinburgh, Scotland
- Olaf Wiest, University of Notre Dame, Notre Dame, Indiana

New Facility Staff

Yanwen Zhang, Senior Research Scientist I, joined the Interfacial & Nanoscale Science Facility.

Publications

Alexandrova AN, AI Boldyrev, HJ Zhai, LS Wang, E Steiner, and PW Fowler. 2003. "Structure and Bonding in B₆⁻ and B₆: Planarity and Antiaromaticity." *Journal of Physical Chemistry A* 107(9):1359-1369.

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