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

Biogeochemistry Grand Challenge Principal Investigators Have First Gathering

The first working meeting of the Biogeochemistry Grand Challenge (BGC) was held in EMSL June 22 and 23. The purpose of the meeting was to engage all investigators on the latest technical progress, as well as enhance the overall coordination, information exchange, and synthesis needed to achieve the BGC's outcomes.

The BGC, which was initiated in December 2005, is a three-year integrated investigation to understand the mechanisms by which bacteria interact with and transfer electrons to the mineral surfaces on which they live. This has implications for environmental remediation and energy production as well as the development of engineered devices. The coordinators are Pacific Northwest National Laboratory (PNNL) senior chief scientists John Zachara and Jim Fredrickson. EMSL staff and resident users involved in the BGC include Michael Bowman, Tim Droubay, Dan Gaspar, Mike Kennedy, Sebastien Kerisit, Brian Lower, Peter Lu, Shuisong Ni, Duohai Pan, Kevin Rosso, and Svetlana Yanina. Other PNNL staff involved include Alex Beliaev, Yuri Gorby, Margie Romine, Liang Shi, and Tjerk Straatsma.

Approximately 35 researchers from 12 institutions heard more than 20 presentations about technical progress, near-term research plans, and how research addresses the BGC's hypothesis—that outer membrane cytochrome(s) MtrC/OmcA are responsible for direct electron transfer to Fe(III) oxide.

The meeting provided the investigators with opportunity to ask questions and discuss issues related to individual research elements within the BGC and to coordinate research efforts, sharing of materials, and collaborative experiments. The results of the meeting will help Zachara and Fredrickson continue developing the roadmap for the BGC.

n-Alkanes on MgO(100)
I. Coverage-Dependent Desorption Kinetics of *n*-Butane
II. Chain Length Dependence of Kinetic Desorption Parameters for Small *n*-Alkanes

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The interactions of an adsorbate with a substrate will determine whether a molecule will react or not. Understanding these complex interactions at a fundamental level may eventually lead to our ability to control the reactivity and selectivity of gas/surface reactions. This research describes a detailed method to model the desorption kinetics of alkanes interacting with an MgO substrate.

The interactions of an adsorbate with a substrate, be it a metal, an oxide or an ice, determine the ultimate fate of that molecule (i.e., whether the molecule scatters, traps, adsorbs, or reacts). Understanding these complex interactions at a fundamental level may eventually lead to our ability to control the reactivity and selectivity of gas/surface reactions. For example, during the last decade much progress has been made in understanding supported metal catalysts at the nanometer scale due to research on model catalyst systems. By studying these model systems, improvements in the efficiency and cleanliness of industrial chemical reactions can be made. Understanding the effect that the nanometer-scale confinement of matter has on catalytic properties is one of the current scientific challenges. Detailed analysis at the nanoscale allows us to probe the atomic scale interactions of the adsorbed metals and their oxide supports, with each other and with other adsorbed species.

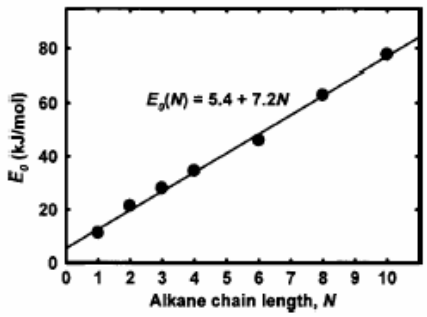

Figure 1. Desorption energy for a series of normal chain alkanes.

Alkane adsorption on oxide surfaces is of significant interest because of the wide use of oxides in heterogeneous catalysts as support materials and as active catalysts. For example, MgO catalysts are used for the oxidative coupling of methane to form C_2 hydrocarbons or for methane oxidation to produce formaldehyde. The MgO(100) surface is one of the most thoroughly studied of all single-crystal oxide surfaces from both experimental and theoretical approaches and has also received significant attention as a support in model catalyst studies. Therefore, the adsorption and desorption kinetics of alkane molecules on MgO and other oxide surfaces is of fundamental interest.

We used molecular beam scattering and temperature programmed desorption (TPD) at low temperatures to study the adsorption and dissociation of hydrocarbons (e.g., methane, ethane, propane) on MgO(100) thin films. Highly collimated molecular beams of the small alkane molecules are impinged on the sample and the adsorption dynamics and desorption kinetics are studied. Figures 1 and 2 show the coverage-dependent desorption energy and desorption prefactor for a series of normal (straight chain) alkanes adsorbed on MgO(100). These values are extracted from a TPD analysis technique that allows the coverage-dependent desorption energy to be accurately determined by mathematical inversion of a TPD spectrum, assuming only that the prefactor is coverage-independent. A variational method is used to determine the prefactor that minimizes the difference between a set of simulated TPD spectra and corresponding experimental data. The data in Figure 1 show that the desorption energy increases linearly with chain length. The data in Figure 2 show that the prefactor for desorption increases dramatically with chain length.

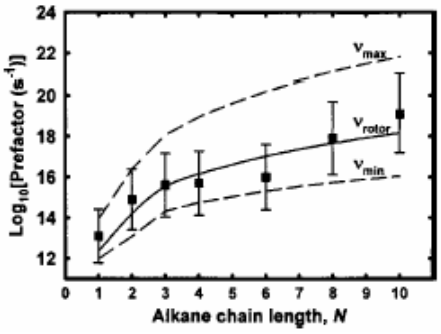

Figure 2. Desorption prefactors for a series of normal chain alkanes.

The observed increase can be physically justified by considering the increase in rotational entropy available to the molecules in the gas-like transition state for desorption. The dashed lines are predictions using various models to calculate the entropic change between a molecule adsorbed on the surface and one in the gas phase.

We have demonstrated the use of an optimization-inversion method for analysis of these TPD data that allows accurate determination of coverage-dependent desorption-kinetics parameters. Using these analysis results, we demonstrated that we are able to accurately simulate the TPD experiments over a wide range of initial coverages and heating rates. These measurements will advance our specific understanding of the catalytic activity of this important combustion catalyst and our general understanding of particle-size effects in hydrocarbon catalysis. Details of this exciting research are published in Tait et al. 2005a and b.

Citations

Tait SL, Z Dohnalek, CT Campbell, and BD Kay. 2005a. "*n*-Alkanes on MgO(100). I. Coverage-Dependent Desorption Kinetics of *n*-butane." *Journal of Chemical Physics* 122(16):164707 (pages 1 - 9).

Tait SL, Z Dohnalek, CT Campbell, and BD Kay. 2005b. "*n*-Alkanes on MgO(100). II. Chain Length Dependence of Kinetic Desorption Parameters for Small *n*-Alkanes." *Journal of Chemical Physics* 122(16):164708 (pages 1 - 13).

Multiscale Modeling of Biochip Systems

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A project has been undertaken that uses multiscale computational techniques to understand the basic physics and chemistry underlying biochip systems. Such systems may be useful for identification of gene mutation, DNA-protein and protein-protein binding, identification of pollutant effects on gene and protein expression, and contaminated water analysis.

Biochip technologies use molecular probes tethered on surfaces for compound analysis. The applications of such technologies are varied and include, but are not limited to, identification of gene mutation, DNA-protein binding, protein-protein-binding, identification of pollutant effects on gene and protein expression, and contaminated water analysis. Many of the experimental phenomena observed in these applications occur on time scales that are outside the reach of explicit atom molecular dynamics simulations. This project proposes the use of multiscale computational techniques to understand the basic physics and chemistry underlying biochip systems.

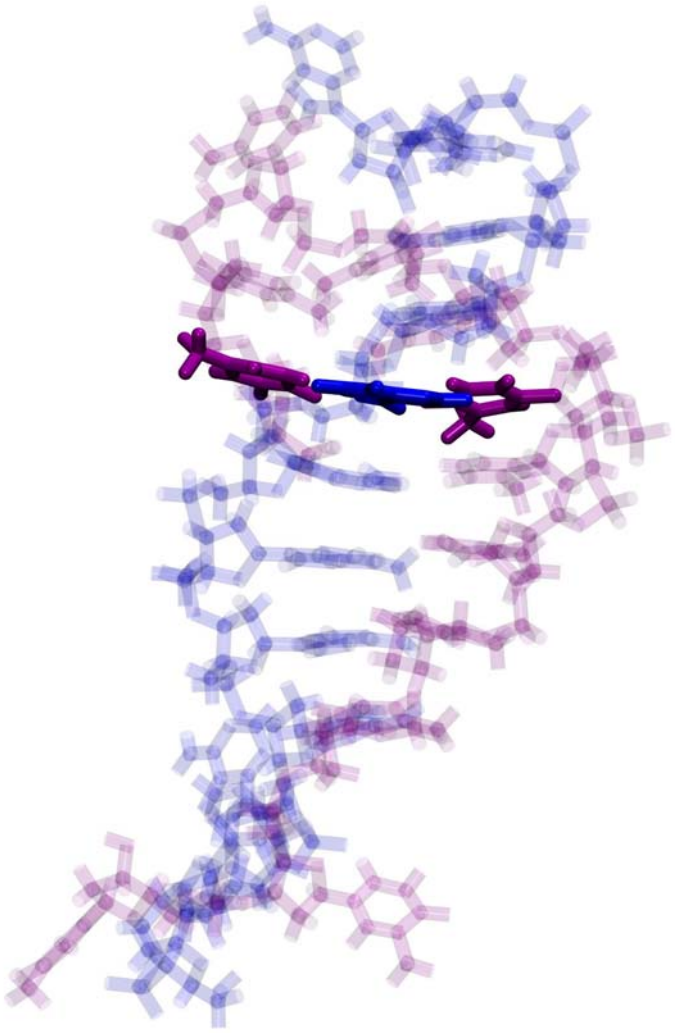

Figure 3. Representation of DNA duplex (translucent) from a snapshot at 10.83 ns. The blue strand is adenine and the red strand is thymine. In the middle region, the thymine (T13) loops back and forms a triplet structure with the adenine (A8, center) and the thymine (T18, right).

The first part of this project focused on the adsorption of single-stranded DNA on a surface. Single-stranded DNA immobilized on a surface has recently become a popular design for biosensors. The properties of the solid-liquid interface are

crucial to both the immobilization of the probe onto the surface and the hybridization of the unknown biomolecule with the target probe. An all-atom molecular dynamics simulation was performed using a 12-base DNA adsorbed onto a 5.1 x 5.3 nm^2 silica surface coated with a layer of positively charged amine groups. Preliminary results reveal that the DNA diffuses to the surface after 40 ns and, once close to the surface, the DNA adopts a more compacted conformation than the free-solution conformation.

To better understand the dehybridization process whereby the duplex unwinds, another molecular dynamics simulation was performed with a duplex DNA strand under melting conditions. Preliminary data show that the ends of the duplex unwind, but total melting does not occur, even after 23 ns. Surprisingly, the system adopts an unusual base-pairing that more closely resembles a Hoogsteen base-pairing for part of the duplex, while the remaining duplex maintains the usual Watson-Crick base-pairings.

Another part of the project focused on protein-DNA complexes. Molecular dynamics simulations of the *Serratia marcescens Endonuclease* monomer with and without DNA were performed. This system exists both as a monomer and a dimer, with both being functional. The results from this simulation revealed that solvent water molecules play an important role. Evaluation of water clusters and pathways in the protein led to the rationalization of a possible mechanism for cleavage of the enzyme.

An investigation into the structural and dynamical solvent properties around hydrophobic solutes was also performed. The mechanism determined for the attractive mean forces between the plates is very different, depending on the nature of the solute-solvent interaction. This has implications for the mechanism of the hydrophobic effect for macromolecules. The focus was shifted to water trapped between the hydrophobic plates, and the results indicated that the translational and reorientational mobilities of water are much slower at the smaller separation and increases as the separation between solutes becomes larger. This behavior is reminiscent of that of water in the vicinity of a macromolecule's surface clefts or trapped between two domains of a macromolecule (Figure 3).

The multiprocessor computing facilities at EMSL were used for all calculations presented. Without these facilities, the long-time simulations needed to discern the mechanisms presented would not have been possible.

Stabilization of Very Rare Tautomers of Uracil by an Excess Electron

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Researchers are studying rare tautomers of nucleic acid bases that are involved in mispairing of nucleic acid bases in DNA and thus in the development of point mutations. This research appeared on the cover of the May 21, 2005, issue of Physical Chemistry Chemical Physics: PCCP.

A tautomer is one of two or more structural isomers—a compound having the same molecular formula but different structures—that exist in equilibrium and are readily converted from one isomeric form to another. Rare tautomers of nucleic acid bases are involved in mispairing of nucleic acid bases in DNA and thus in the development of point mutations. PNNL scientists, in collaboration with researchers from the University of Gdansk and Adam Mickiewicz University, are uncovering a molecular pathway of destruction of the six-member ring structure of pyrimidine bases by low-energy electrons. In the current work, the scientists focused on chemical transformations of nucleic acid bases induced by low-energy electrons. Figure 4 shows a possible mechanism of destruction of the six-member ring structure; this graphic appeared recently in Bachorz et al. 2005.

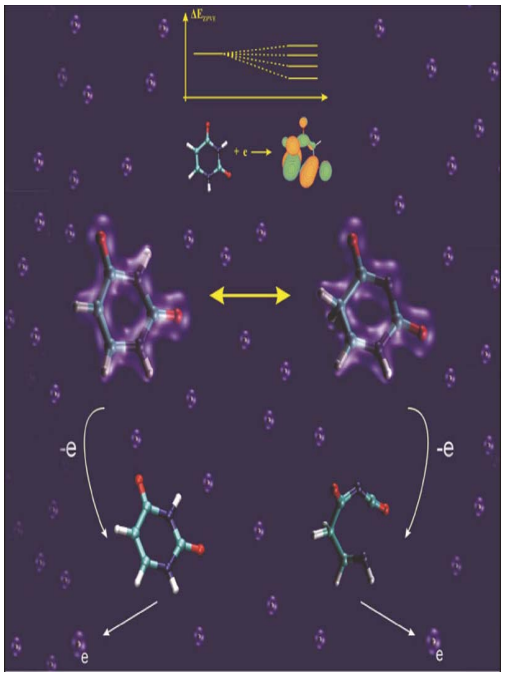

Figure 4. This graphic shows a possible mechanism of destruction of the six-member ring structure of uracil and appeared on the cover of the May 21, 2005, issue of *Physical Chemistry Chemical Physics*.

The principal finding of this research is that low-energy electrons favor very unusual tautomers of nucleic acid bases. These are not canonical or conventional rare tautomers, in which proton transfer takes place between electronegative atoms nitrogen or oxygen. Instead, the most stable anionic tautomers result from enamine-imine transformation—where a proton is transferred from a nitrogen atom to a carbon atom. These new tautomers might affect the structure and properties of DNA and RNA. In particular, they undergo a barrier-free decomposition of the ring structure of a nucleic acid base upon an excess electron detachment (this is what is shown on the cover). These decompositions might be viewed as lesions to DNA or RNA. The new anionic tautomers might contribute to the

chemistry of RNA and DNA exposed to low-energy electrons in condensed-phase environments. The researchers will continue to explore this problem.

This research is funded by DOE's Low-Dose Radiation Research Program, which supports fundamental science to determine health risks from exposures to low levels of radiation. DNA damage from radiation-induced mutation is potentially a critical pathway to adverse health effects. For example, single- and double-strand breaks in DNA are induced by lesions formed by low-energy electrons, which are produced in copious amounts by high-energy radiation. The molecular mechanism forming these lesions is not yet known.

Citation

Bachorz RA, J Rak, and MS Gutowski. 2005. "Stabilization of Very Rare Tautomers of Uracil by an Excess Electron." *Physical Chemistry Chemical Physics: PCCP* (10):2116 – 2125.

Protein Expression Profiling of Wild-Type *Caenorhabditis elegans* during Development

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(a) University of British Columbia, Vancouver, British Columbia, Canada

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Understanding how different cell types, such as skin and nerve cells, are created from the same genome is one of biology's great unsolved mysteries. This work will describe proteins of individual cell types during the development in C. elegans. The data obtained in this study will be combined with other existing information to provide details of protein expression profiles and an increased understanding of how different cells are generated from the same genome.

Proteomics is the leading technology used for high-throughput analysis of protein expression on a genome-wide scale. The availability of complete genomic sequences and technologies that allow comprehensive analysis of global expression profiles of messenger RNA have greatly expanded our ability to monitor the internal state of a cell. However, biological systems need to be explained in terms of their protein activity, as mRNA by itself is an imperfect monitor of cellular activity. In development, much gene regulation occurs post-transcriptionally, and these levels of gene regulation are inaccessible when one studies only steady-state levels of transcripts. A study of the proteome of *C. elegans*, an organism with a sequenced genome and extensive data on whole animal and specific cellular mRNA expression, is an excellent test case for current proteome technology. In one case, the identification of a protein in a tissue where a transcript has been identified will affirm the expression of the gene in that tissue. On the other hand, we, as well as others, have identified thousands of transcripts within a tissue or a given cell type. This data will provide a benchmark to measure the success and sensitivity of the proteomics approach.

Currently, we are investigating protein expression patterns in the 550 cell whole embryo and isolated FAC sorted myo-3::GFP labeled muscle cells. The transcriptomes for each of these test samples are rich, extending to many thousands of different genes. We are using a

combination of enzymatic digestion, high-resolution liquid chromatography-Fourier transform ion cyclotron resonance mass spectrometry (LC-FTICR) and the accurate mass and time (AMT) tag strategy to build a snapshot of the proteome in these two samples. Initially, a peptide mass and time tag database was generated using tandem mass spectrometry (MS/MS) following extensive multidimensional LC separations, and this database will serve as a 'look-up' table for peptide identification in all subsequent studies. The generation of an AMT tag database largely obviates the need for subsequent MS/MS analyses and thus should facilitate high-throughput analyses. Furthermore, the higher sensitivity of the FTICR analysis will increase sampling depth, allowing detection of low-abundance proteins in the complex and small-sized samples. This approach will allow us to gain a detailed picture of not only the whole embryo proteome, but also individual cellular proteomes.

For generating the AMT tag database, proteins from the readily available wild-type embryo lysates were digested, fractionated, and analyzed using LC-MS/MS, resulting in identification of 19,803 different peptides covering 4,297 proteins. Eighty percent of these proteins were in concordance with the 7,000 different genes found expressed in the embryo (SAGE data); thus, this AMT tag database will provide a solid foundation for proceeding with high-throughput and highly sensitive proteome profiling of individual cell types. Proteins isolated from 580,000 muscle cells (with a cell diameter of only 1/10 of that of a typical mammalian cell) isolated by FACS analysis of disrupted embryos were digested and directly analyzed using a single LC-FTICR analysis. As a result, more than 1,000 muscle proteins were identified by searching the FTICR data in the AMT tag database (Figure 5). In addition, we were able to identify a large number of predicted and partially confirmed proteins from both embryos and muscle cells.

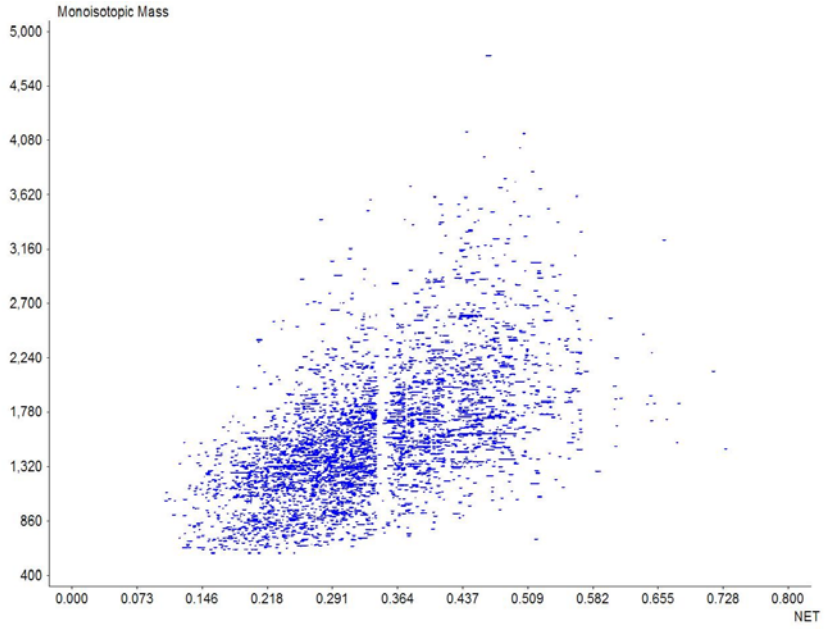
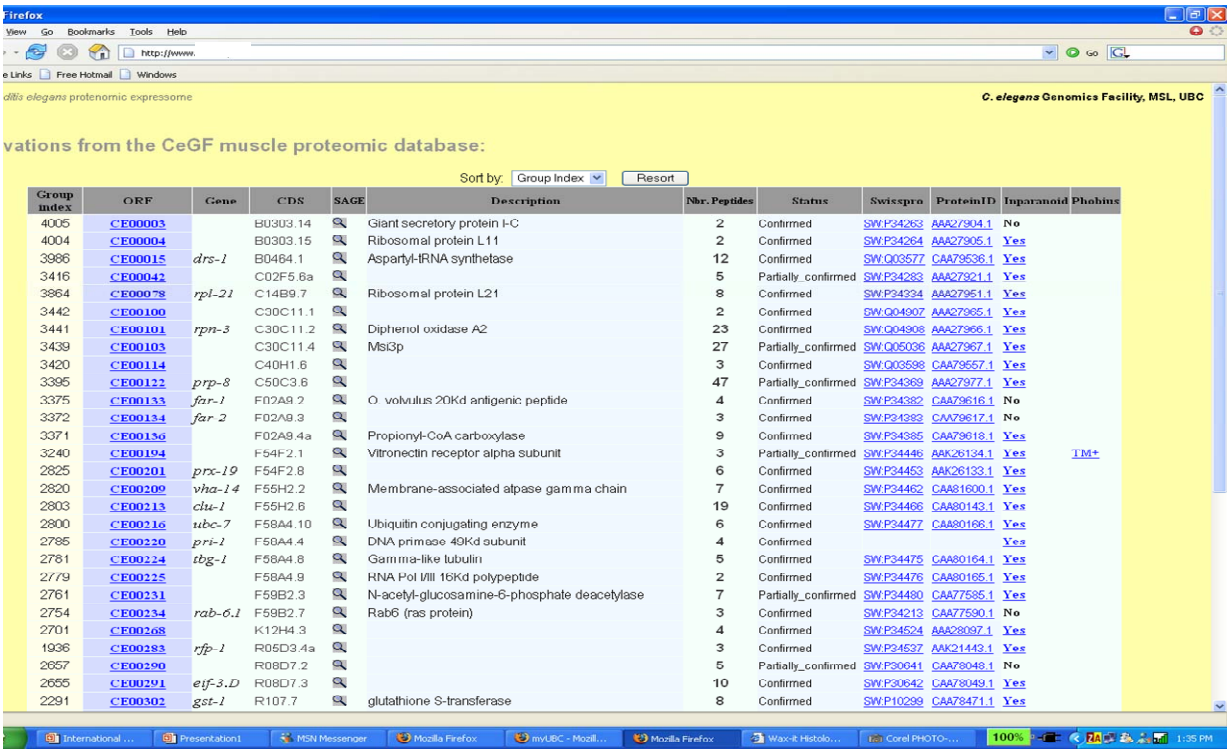


Figure 5. Two-dimensional display of LC-FTICR analysis of the tryptic peptides from 580,000 isolated FAC sorted myo-3::GFP labeled muscle cells. Over 3000 different peptides covering 1071 non-redundant proteins were identified.

A *C. elegans* proteome database (Figure 6) will be soon available.



Group index	ORF	Gene	CDS	SAGE	Description	Nbr. Peptides	Status	Swissprot	ProteinID	Inparanoid	Phobius
4005	CE00003		B0303.14		Giant secretory protein I-C	2	Confirmed	SW:P34263	AAA27904.1	No	
4004	CE00004		B0303.15		Ribosomal protein L11	2	Confirmed	SW:P34264	AAA27905.1	Yes	
3986	CE00015	drs-1	B0464.1		Aspartyl-tRNA synthetase	12	Confirmed	SW:Q03577	CAA79536.1	Yes	
3416	CE00042		C02F5.6a			5	Partially_confirmed	SW:P34283	AAA27921.1	Yes	
3864	CE00078	rpl-21	C14B9.7		Ribosomal protein L21	8	Confirmed	SW:P34334	AAA27951.1	Yes	
3442	CE00100		C30C11.1			2	Confirmed	SW:Q04907	AAA27965.1	Yes	
3441	CE00101	rpn-3	C30C11.2		Diphenol oxidase A2	23	Confirmed	SW:Q04908	AAA27966.1	Yes	
3439	CE00103		C30C11.4		Msi3p	27	Partially_confirmed	SW:Q05036	AAA27967.1	Yes	
3420	CE00114		C40H1.6			3	Confirmed	SW:Q03598	CAA79557.1	Yes	
3395	CE00122	prp-8	C50C3.6			47	Partially_confirmed	SW:P34369	AAA27977.1	Yes	
3375	CE00133	far-1	F02A9.2		O. volvulus 20Kd antigenic peptide	4	Confirmed	SW:P34382	CAA79616.1	No	
3372	CE00134	far-2	F02A9.3			3	Confirmed	SW:P34383	CAA79617.1	No	
3371	CE00136		F02A9.4a		Propionyl-CoA carboxylase	9	Confirmed	SW:P34385	CAA79618.1	Yes	
3240	CE00194		F54F2.1		Vitronectin receptor alpha subunit	3	Partially_confirmed	SW:P34446	AAK26134.1	Yes	TM+
2825	CE00201	prx-19	F54F2.8			6	Confirmed	SW:P34453	AAK26133.1	Yes	
2820	CE00209	vha-14	F55H2.2		Membrane-associated alpase gamma chain	7	Confirmed	SW:P34462	CAA81600.1	Yes	
2803	CE00213	clu-1	F55H2.6			19	Confirmed	SW:P34466	CAA80143.1	Yes	
2800	CE00216	ubc-7	F58A4.10		Ubiquitin conjugating enzyme	6	Confirmed	SW:P34477	CAA80166.1	Yes	
2785	CE00220	pri-1	F58A4.4		DNA primase 49Kd subunit	4	Confirmed			Yes	
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2754	CE00234	rab-6.1	F59B2.7		Rab6 (ras protein)	3	Confirmed	SW:P34213	CAA77590.1	No	
2701	CE00268		K12H4.3			4	Confirmed	SW:P34524	AAA28097.1	Yes	
1936	CE00283	rfp-1	R05D3.4a			3	Confirmed	SW:P34537	AAK21443.1	Yes	
2657	CE00290		R08D7.2			5	Partially_confirmed	SW:P30641	CAA78048.1	No	
2655	CE00291	eif-3.D	R08D7.3			10	Confirmed	SW:P30642	CAA78049.1	Yes	
2291	CE00302	gst-1	R107.7		glutathione S-transferase	8	Confirmed	SW:P10299	CAA78471.1	Yes	

Figure 6. *C. elegans* proteome database.

Detection and Characterization of ZSM-5 in a Mesoporous Host Matrix

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(c) Universite' Pierre et Marie Curie, Paris, France

In this work, ultrahigh-field ^{27}Al magic-angle spinning and multiple quantum magic-angle spinning nuclear magnetic resonance spectrometries have proven to be essential tools for the detection of zeolite nanoclusters and the different aluminum environments in nanozeolite/mesoporous aluminosilicate composites. Demonstration of the presence of zeolite nanoclusters in these composites is the first step in evaluating their potential as a catalyst of the future—critical for converting crude oil into gasoline and other petroleum products.

Zeolites are catalysts that are critical for converting crude oil into gasoline and other petroleum products; without them, many fuels and petrochemicals would not be readily available. Future improvements in catalyst performance require a good understanding of their internal structure. While methodologies such as x-ray diffraction and Fourier transform infrared (FTIR) spectroscopy have provided limited structural information, nuclear magnetic resonance spectroscopy (NMR) has given the most detailed insights. In order to obtain the high-quality data needed for structure determination, higher magnetic

fields are needed, such as the 750- and 800-MHz spectrometers available at EMSL. Data collected at 500 MHz has proven useful, but not all of the aluminum atoms present can be detected at this field.

Zeolites are very open frameworks of aluminosilicates or silicates composed of corner- and edge-sharing SiO_4^{4-} and AlO_4^{5-} tetrahedra. They contain regular systems of cavities and channels of molecular dimensions, which control the uptake of organic molecules in terms of shape and size selectivity. Zeolites are powerful acid catalysts, but their small pores limit diffusion, which in turn limits the speed of catalysis. Improvement in catalytic rates would bolster the efficiency of the oil refining industry. It has been shown recently that the coating of protozeolitic nanoclusters onto the surface of preformed mesostructured aluminosilicates can greatly improve their hydrothermal stability and acidity, both essential for catalysis (Figure 7). Although FTIR observations confirm the presence of zeolite nanoclusters in the mesopore channels, x-ray diffraction diagrams fail to indicate the presence of zeolite crystals in the coated material. Ultrahigh-field (17.6 T) ^{27}Al magic-angle spinning (MAS) and multiple quantum magic-angle spinning (MQMAS) NMR were used to detect the zeolite nanocrystals and quantify the multiple aluminum environments in these materials. A complete account is given in Do et al. 2004.

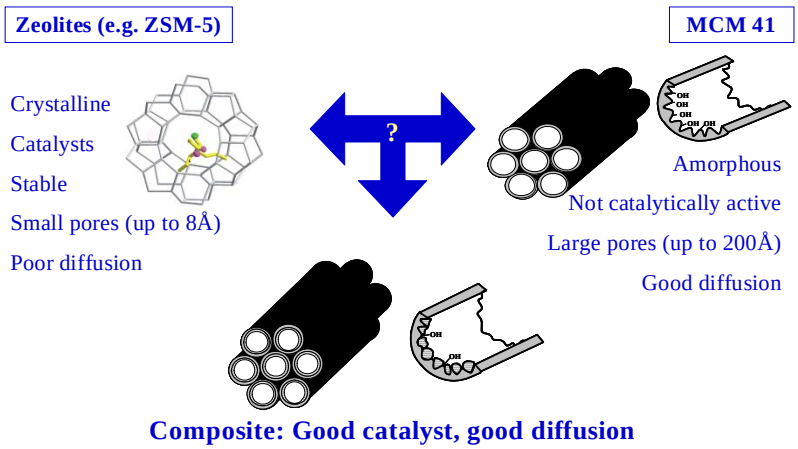

Figure 7. The incorporation of zeolite nonacrystals in the mesoporous structure.

Figure 8a shows the various aluminum environments detected by ^{27}Al MAS NMR at 17.6 T. The parent sample shows two broad peaks (one tetrahedral and the other octahedral) characteristic of amorphous materials, and the calcined zeolite-coated samples show two additional sharper peaks consistent with the chemical shift values of the corresponding zeolite. The broadening of these peaks, compared to the ones obtained from perfectly crystalline zeolites, results from their being in a less ordered environment. As Figure 8b shows, it is possible to discriminate the higher degree of ordering of the zeolite (longer T2) from the amorphous mesoporous framework (shorter T2) through a series of spin echo

experiments. ^{27}Al MQMAS NMR confirms these results, as only two partially resolved signals are observed, which have been assigned to the tetrahedral aluminum sites in the zeolite (Figure 8c).

Ultrahigh-field ^{27}Al MAS and MQMAS NMR have proven to be essential tools for the detection of zeolite nanoclusters and the different aluminum environments in nanozeolite/mesoporous aluminosilicate composites, as these features cannot be detected by conventional x-ray diffraction techniques. The demonstration of the presence of zeolite nanoclusters in these composites is the first step in evaluating their potential as a catalyst of the future.

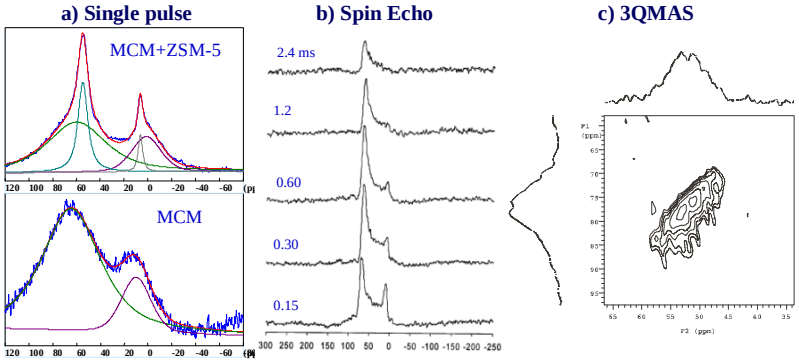

Figure 8. The use of ultrahigh field ^{27}Al NMR to discriminate the nanozeolite from the mesostructure.

Citations

Do Trong-on, A Nossov, MA Springuel-Huet, C Schneider, JL Bretherton, CA Fyfe, S Kaliaguine. (2004) "Zeolite Nanoclusters Coated onto the Mesopore Walls of SBA-15." *Journal of the American Chemical Society* 126(44):14324-14325.

Defect Configuration and Relaxation in 4H Silicon-Carbide

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(a) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington
(b) Pacific Northwest National Laboratory, Richland, Washington

The wide band gap semiconductor silicon carbide (SiC) has remarkable physical, chemical, and electronic properties that make it very attractive for high-speed communications and high-temperature, high-frequency, and high-power applications. Doping SiC material is necessary for these applications, and ion implantation can be used effectively for doping. This study investigates the effects induced by ion irradiation in SiC.

Ion implantation is the only planar, selective-area doping technique available for SiC, since the diffusion coefficients of impurities in SiC are negligibly small at or below 1800 K. Ion implantation, however, inevitably produces a significant concentration of defects and lattice disorder, which lead to a growth of secondary defects or other polytype structures during post-implantation annealing or high-temperature operation. Failure of prototype devices is often associated with point defects or larger agglomerates of point defects formed by the implantation process or during post-implantation annealing. One of the critical issues for SiC device fabrication is to understand defect configuration, relaxation, and annihilation following annealing. Irradiation-induced defects are studied for both the silicon and carbon sublattices in 4H-SiC under 2 MeV gold ion irradiation at 165 K in 4H-SiC using ion channeling techniques along two crystallographic directions (Figure 9).

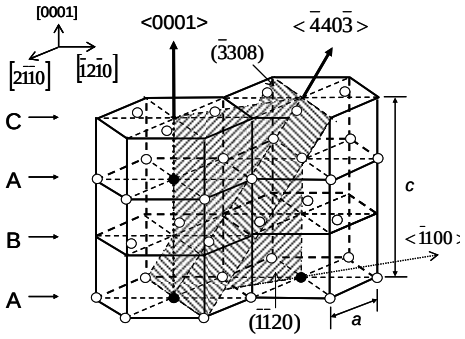

Figure 9. The first stacking sequence of the silicon sublattice in 4H-SiC with the axes <0001> and <4403> indicated. The filled symbol is used when the silicon atom is on the corresponding axis.

Molecular dynamics simulations on defect evolution in SiC under ion irradiation indicate that energetic ions primarily produce interstitials, monovacancies, antisite defects, and small defect clusters within collision cascades. In covalent SiC, dumbbell interstitials are important defects due to their low formation energies, as shown in Figure 10. In addition to dumbbell interstitials, there are other possible single interstitial configurations. For example, the seven carbon interstitial configurations are illustrated in Figure 11. The molecular dynamics results demonstrate that most single interstitial configurations are formed on the silicon-carbon dimer rows that are parallel to the <0001> direction. When aligning the probe beam along the <0001> direction, the D_1 and D_2 dumbbell interstitials and the C_H and Si_H type single interstitials can be detected. The other single interstitial configurations are shielded from the analysis beam by the silicon-carbon rows along the <0001> direction, and therefore will not contribute to the backscattering/reaction yield. On the other hand, along the <4403>

direction, all seven possible configurations for the single interstitials and all the dumbbell interstitials are accessible to the probe beam used for Rutherford backscattering spectroscopy and ^{12}C $(d,p)^{13}C$ nuclear reaction analysis. Because all interstitial configurations contribute to the backscattering along the $<\bar{4}40\bar{3}>$ direction, a significantly higher relative disorder is observed on both the silicon and carbon lattices along this direction.

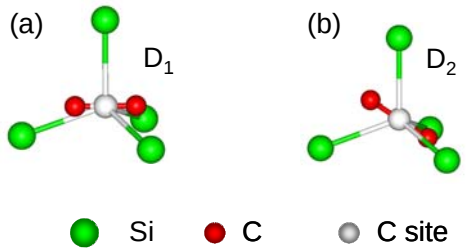

Figure 10. Fundamental structure of dumbbell interstitials: (a) D_1 and (b) D_2. The light gray spheres and cylinders show the tetrahedron in the ideal lattice.

After completion of the channeling measurements for the as-implanted samples, isochronal annealing was carried out sequentially at temperatures from 200 to 870 K. The relative residual disorder for the higher dose samples at the damage peak for both the silicon and carbon sublattices was determined along both directions after each annealing. The relative increase at 200 K along the $<\bar{4}40\bar{3}>$ direction, particularly for the carbon sublattice, is associated with the relaxation of defects to lower-energy configurations that give an increased contribution to the backscattering. As the annealing temperature further increases, the residual disorder decreases along both the <0001> and $<\bar{4}40\bar{3}>$ directions. At higher annealing temperatures, interstitials will migrate, resulting in annihilation or clustering. This leads to a decrease in the concentration of local defects and some defect-stimulated epitaxial recrystallization of amorphous domains. Above room temperature, there is a recovery stage at ~500 K that is more pronounced for high-dose samples. This recovery stage is not observed by positron lifetime spectroscopy, which suggests that vacancy defects are unaffected by the recovery process at these temperatures.

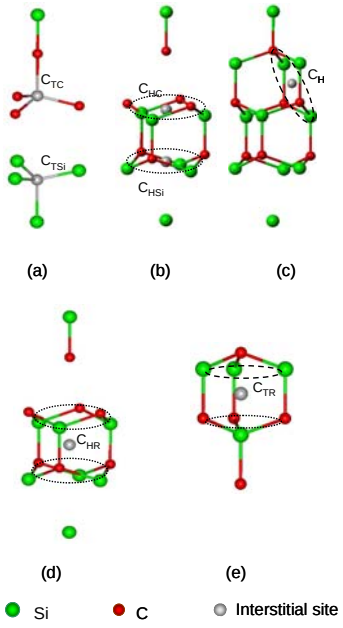

Figure 11. Seven possible positions for carbon single interstitials, two tetrahedral positions on the long row as (a), three hexagonal positions as (b) and (c), and two highly symmetric interstitial structures, as (d) between the two hexagonal Si_3C_3 rings on the long row and (e) between a trigonal Si_3 and a trigonal C_3 rings on the short row.

Complete recovery of the residual disorder is not observed on either sublattice or along either direction after annealing up to 870 K due to residual amorphous domains and stable defect clusters. Thermal annealing at 1300 K or higher is necessary for complete restoration of the crystalline order.

Nitrogen Analysis Using Energetic Ion Beams

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(a) Pacific Northwest National Laboratory, Richland, Washington
(b) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

As a special case of nuclear reaction analysis, nuclear elastic scattering analysis (or non-Rutherford scattering analysis) is one of the important methods in ion-beam analysis, and it is the preferred technique to analyze light elements in a heavy matrix. In order to quantify the light elements, the cross sections of the elements need to be established to perform the nuclear elastic scattering analysis. This study reports cross sections for $^{14}N(p,p)^{14}N$ and $^{14}N(\alpha,\alpha)^{14}N$ at a scattering angle of 150° in the laboratory system.

The excitation curves for $^{14}N(p,p)^{14}N$ in the proton energy range from 2.480 to 3.230 MeV are shown in Figure 12. Both the data from this experiment at θ_{Lab} = 150° and the data of Bashkin et al. 1959 for θ_{Lab} = 159.5° show a sharp nuclear resonant peak at ~3.2 MeV. The peak intensity and full width at half maximum (FWHM) at 150° correspond to 24σR and 20 keV, respectively. Although the FWHM is small, this width corresponds to ~900 nm in materials like GaN due to the small stopping powers of the energetic protons. For this reason, analysis of ^{14}N in solids can be performed around the resonant peak over a small range of energy (ΔE ≈ 5 keV) at 150°, where the variation of the scattering cross sections is ~10%. Besides the resonance, there is also a cross section plateau (~6.8σR) over a wide range of energy from 2.48 to 3.15 MeV for elastic scattering at 150°. The energy width (~700 keV) of the plateau corresponds to a depth of ~28 μm for GaN, based on the SRIM-2003 database. This plateau can be used to quantify the ^{14}N (total content) in solids. However, for conventional ion-beam analysis using surface-barrier detectors, this cross-section plateau is not strongly recommended for profiling ^{14}N, since the depth resolution is poor, on the order of 150 nm. For He^+ elastic scattering from ^{14}N, the cross-section data are shown in Figure 13 for θ_{Lab} = 150° (this experiment) and θ_{Lab} = 165°(from Feng et al. 1994). At a scattering angle of 150°, the cross section decreases gradually from 2σR to σR with increasing ion energy over the range between 3.144 and 3.505 MeV. At 3.565 MeV, there is a small resonant peak (1.96σR), followed by a stronger nuclear resonance located at 3.686 MeV, with the peak maximum of 4.82σR.

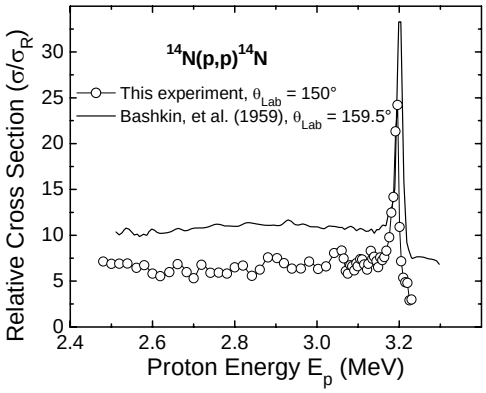

Figure 12. Cross section of H^+ backscattering from ^{14}N at 150° as a function of ion energy. Also included are the data at θ_{Lab} = 159.5° from Bashkin et al. 1959.

Although the resonant peak positions of the two data sets agree well, the intensity of the cross sections at the larger peak is greatly reduced from 8.9σR at 165° to 4.82σR at 150°. In both cases, the enhancement of the cross section is relatively small as compared to the proton scattering shown in Figure 12. The resonant peak at 3.686 MeV has a FWHM of ~100 keV at 150°. Compared with the $^{14}N(p,p)^{14}N$ elastic scattering at 150°, the $^{14}N(\alpha,\alpha)^{14}N$ scattering has a much better depth resolution (~25 nm for GaN at the surface), but the probing depth is greatly reduced (~120 nm starting from GaN surface with allowance of a 10 percent variation in cross section at the peak). The lower cross-section values of the $^{14}N(\alpha,\alpha)^{14}N$ scattering make it less favorable to analyze the total content of ^{14}N in solids as compared to the $^{14}N(p,p)^{14}N$ scattering shown in Figure 12.

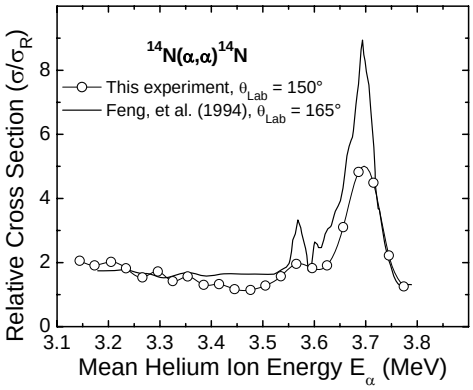

Figure 13. Cross section of He^+ backscattering from ^{14}N at 150° as a function of ion energy. Also included are the data at θ_{Lab} = 165° from Feng et al. 1994.

As an example to illustrate nitrogen analysis based on the measured scattering cross sections, a GaN single crystal film on an Al_2O_3 substrate was analyzed in channeling geometry along the <0001> axis (close to the surface normal). The specimen was irradiated with 1.0 MeV Au^{2+} ions to a fluence of 1.5 ions/nm2 at 150 K. Conventional 2.0 He^+ Rutherford backscattering/channeling analysis leads to a broad damage peak on the gallium sublattice; however, the scattering signals from ^{14}N are completely buried by the high intensity of the gallium spectrum. Such a spectrum does not allow for the study of the nitrogen sublattice in GaN. Figure 14 shows the results from the 3.746 MeV He^+ non-Rutherford backscattering/channeling for the same sample. Clearly, the damage peaks on both the gallium and nitrogen sublattices in GaN appear in the spectrum. Based on a slightly higher energy (3.8 MeV) of He^+ ions, the accumulation of disorder on both the gallium and nitrogen sublattices in wurtzite GaN has been studied as a function of ion fluence.

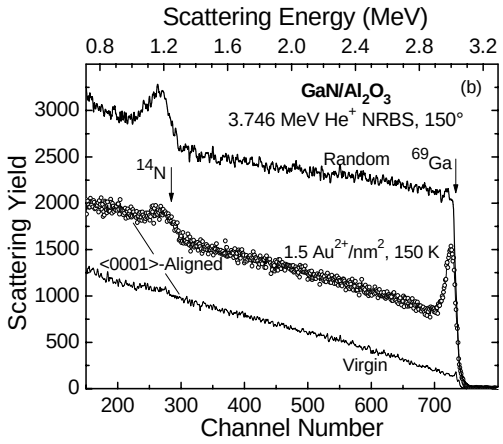

Figure 14. A typical example showing the energy spectra of 3.746 MeV He^+ non-Rutherford backscattering/channeling for a GaN film on a sapphire substrate.

Citations

Bashkin S, RR Carlson, and RA Douglas. 1959. "Cross Section for Elastic Scattering of Protons by N^{14}." *Physical Review* 114(6):1552-1553.

Feng Y, Z Zhou, G Zhou, and F Yang. 1994. "Cross-Sections for 165° Backscattering of 2.0 – 9.0 MeV ^{4}He Ions from Nitrogen." *Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms* 94:11.

Reoxidation of Reduced Uranium with Iron(III) (Hydr)Oxides under Sulfate-Reducing Conditions

RK Sani,[(a)] BM Peyton,[(a)] A Dohnalkova,[(b)] and JE Amonette[(b)]

(a) ***Washington State University, Pullman, Washington***

(b) ***Pacific Northwest National Laboratory, Richland, Washington***

Thousands of sites across the United States contain high levels of uranium contaminants generated by mining and processing activities. Understanding uranium precipitation by metal-reducing bacteria may lead to improvements in bioremediation processes.

Uranium is the most common radionuclide in soils, sediments, and groundwater at DOE sites across the nation and therefore is of particular environmental concern. The most common form of uranium in groundwater is typically U(VI), which is present either as the uranyl cation, schoepite, or as anionic carbonate complexes. Removal of U(VI) from solution can occur by sorption, precipitation as a U(VI) compound, or reductive precipitation as a U(IV) compound. Although sorption of U(VI) can control aqueous concentrations of uranium under oxidizing conditions, the reversibility of such a process makes reductive precipitation more desirable. *In situ* microbial reduction of U(VI) to form U(IV) precipitates of uraninite may be an attractive alternative strategy for remediation of uranium-contaminated subsurface environments. It is vital, therefore, to identify and characterize processes that control the stability of uranium to restrict its environmental risk.

Knowledge of U(VI) reduction by sulfate-reducing bacteria under microbial growth conditions is limited. *In situ* stimulation of anaerobic microbial metal-transformation processes may be an effective treatment alternative to immobilize heavy metals and radionuclides. More research is needed, however, to better understand interactions of sulfate-reducing bacteria, metal, radionuclide contaminants, and mineral phases in the subsurface.

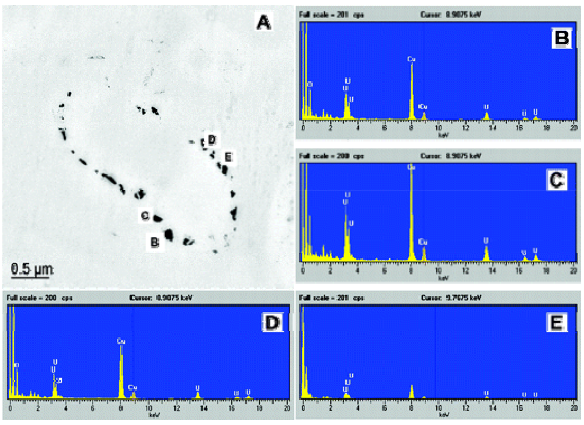

Figure 15. (A) Transmission electron microscopy image of an unstained thin section of *D. desulfuricans* G20 treated with U(VI) and hematite showing an oblique section of a bacterium. (B-E) Evident precipitates of biogenic uraninite associated with the cell surfaces were confirmed by energy dispersive spectroscopy and selected area electron diffraction.

X-ray absorption near-edge spectroscopy performed at Argonne National Laboratory and high-resolution transmission electron

microscopy performed at EMSL were used to analyze microbially reduced uranium particles. The results provide evidence that *D. desulfuricans* G20 reduced U(VI) to form nanoparticulate uraninite (Figure 15). Further, results indicate that the type and amount of iron(III) (hydr)oxide present and the type of pH buffer (PIPES or bicarbonate) had significant effects on the rate of U(VI) reduction. After depletion of lactate required for microbial U(VI) reduction, the rate and extent of U(IV) reoxidation were dependent on the type and amount of iron(III) (hydr)oxide present. These results suggest that application of long-term bioimmobilization of uranium must consider additional complexity in processes and reactions, since sulfate and sulfate-reducing bacteria are commonly found in many uranium-contaminated aquifers. Failing to maintain sufficient organic substrate concentrations until available Fe(III) is reduced could lead to unfavorable consequences for the long-term stability of immobilized uranium.

This research is further described in Sani et al. 2005.

Citation

Sani RK, BM Peyton, A Dohnalkova, and JE Amonette. 2005. "Reoxidation of Reduced Uranium with Iron(III) (Hydr)Oxides under Sulfate-Reducing Conditions." *Environmental Science and Technology* 39(7):2059-2066.

Kinetic Evidence for Five-Coordination in $AlOH_{(aq)}^{2+}$ Ion

TW Swaddle,[(a)] J Rosenqvist,[(b)] P Yu,[(b)] EJ Bylaska,[(c)] BL Phillips,[(d)] and WH Casey[(b)]

(a) University of Calgary, Calgary, Alberta, Canada
(b) University of California, Davis, California
(c) Pacific Northwest National Laboratory, Richland, Washington
(d) State University of New York, Stony Brook, New York

Determination of the structure of aluminum in solution in the critical biochemical and geochemical range pH 4-7 is important because its chemical properties, such as aqueous speciation and ligand substitution kinetics, govern aluminum's toxicity towards plants, fish, and humans.

Aluminum ions are important in natural bodies of water because of its potential health affect on plants and fish, but the structure of their coordination shell is a complex unsolved problem. In strong acid (pH < 3.0), Al-III exists almost entirely as the octahedral $Al(H_2O)_6^{3+}$ ion, whereas in basic conditions (pH > 7), a tetrahedral $Al(OH)_4^-$ structure prevails. In the biochemically and geochemically critical pH range of 4.3 to 7.0, the ion structures are less clear. Other hydrolytic species, such as

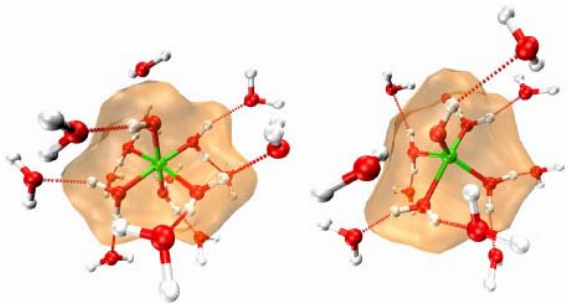

Figure 16. Snapshot of the initial $Al(H_2O)^{63+}$ geometry (left) and the five-coordinate $AlOH^{2+}$ ion (right) that forms in the Car-Parrinetto molecular dynamics simulations.

$AlOH_{aq}^{2+}$, exist and are traditionally assumed to be hexacoordinate.

High pressure ^{17}O-nuclear magnetic resonance (obtained at the University of California, Davis, and State University of New York, Stony Brook) showed, however, that the kinetics of proton and water exchange on aqueous Al-III, coupled with Car-Parrinetto simulations performed using EMSL's 11.8-teraflop supercomputer, supported a five-coordinate $Al(H_2O)_4(OH)^{2+}$ ion as the predominant form of $AlOH_{(aq)}^{2+}$ under ambient conditions (Figure 16). This result contrasts Al-III with other trivalent metal aqua ions for which there is no evidence for stable pentacoordinate hydrolysis products.

This work is further described in Swaddle et al. 2005.

Citation

Swaddle TW, J Rosenqvist, P Yu, E Bylaska, BL Philiips, and WH Casey. 2005. "Kinetic Evidence for Five-Coordination in $AlOH_{(aq)}^{(2+)}$ Ion." *Science* 308(5727):1450-1453.

Awards and Recognition

EMSL User Elected to International Academy of Quantum Molecular Science. Michel Dupuis (Figure 17), an EMSL user and Laboratory Fellow, was elected to the International Academy of Quantum Molecular Science at its 42nd annual meeting held July 2-3, 2005, in Menton, France. Dupuis is part of several EMSL Computational Grand Challenge projects that are running calculations on the Molecular Science Computing Facility's supercomputer.

Figure 17. Michel Dupuis.

The Academy was created in Menton in 1967. Originally, it was limited to 25 regular members under the age of 65, with no limit on senior members. However, the Academy has expanded to 35 regular members under the age of 65 and currently includes 88 members worldwide. Members are selected among scientists from all countries who have distinguished themselves in the broad field of the application of quantum mechanics to the study of molecules and macromolecules. The main goal of the Academy is to provide a forum for international contact and collaboration and a periodical evaluation of the main developments, advances, and promising directions of research in the broad field of its interest.

Patent Award. U.S. Patent 6,911,649, "Particle Generator," was issued on June 28, 2005, to Wayne P. Hess and Alan G. Joly, Pacific Northwest National Laboratory, Richland, Washington; EMSL researcher Kenneth M. Beck; Daniel P. Gerrity, Reed College, Portland, Oregon; and Peter V. Sushko and Alexander L. Shlyuger, University College London, London, United Kingdom.

Professional/Community Service

V.I Goldschmidt Conference. The 15th Annual V.I. Goldschmidt Conference, an annual meeting in geochemistry and mineralogy, was held May 20 through 25 in Moscow, Idaho. Several EMSL staff members, users, and scientific consultants presented research.

Environmental Spectroscopy Symposium. Nancy Foster-Mills, Environmental Spectroscopy and Biogeochemistry Facility Technical Group Leader, organized a symposium on environmental spectroscopy that focused on presentations related to the application of various optical spectroscopies in environmental research. The symposium was held at the Northwest Regional Meeting of the American Chemical Society on June 15 through 18, 2005, in Fairbanks Alaska.

PNNL Family Day. On June 18, EMSL opened its doors as part of PNNL's Family Day, part of PNNL's year-long celebration of its 40th year of operation. Several EMSL staff participated in the days events, giving scientific demonstrations, leading tours, and answering questions to the hundreds of guests visiting the user facility.

Major Facility Upgrades

Kratos Axis Surface Analytical Instrument. The Auger electron spectroscopy function of the Kratos Axis Surface Analytical instrumentation has been inactive for some time. A Kratos representative recently spent nearly two weeks to bring the function back online.

News Coverage

EMSL Grand Challenges. The PNNL press release "Scientists team up for multiyear studies of microbial mysteries" (http://www.pnl.gov/news/2005/05-37.stm) highlighted the launch of the EMSL Grand Challenges, focusing on the work that has begun on both the Biogeochemistry Grand Challenge and the Membrane Biology Grand Challenge.

ScalaBLAST. The PNNL press release "Genomic sequences processed in minutes, rather than weeks" (http://www.pnl.gov/news/2005/05-45.stm) features ScalaBLAST, a sophisticated sequence alignment tool that can divide the work of analyzing biological data into manageable fragments so that large data sets can run on many processors simultaneously.

Visitors and Users

Chemistry and Physics of Complex Systems Facility

- Hashim Ali, University of Iowa, Iowa City, Iowa, gave the seminar "Laboratory Studies of Atmospheric Particles: Heterogeneous Reactions and Phase Transitions."

- Ben Arthurs, Washington State University, Pullman, Washington, worked on microscopy automation of scoring low-dose radiation responses in a green fluorescent protein-based vector.

- Olexandr Bondarchuk, University of Texas at Austin, Texas, worked on the study "Atomically Resolved Studies of Transition Metal Oxides."

- Mingdong Cai, Washington State University, Pullman, Washington, worked on the study "Martensitic Transformations in Shape Memory Alloys by Real-Time Measurement of Surface Work Function Change."

- Todd Engstrom, University of Texas at Austin, Austin, Texas, worked on the study "Condensed Phase Chemical Physics of Low Temperature Amorphous Solids and Gas S urface Interactions.

- Shaun Garland, Shasta College, Redding, California, worked on the study "Characterization of Functional Nanoscale Materials for Vapor Sensing."

- Jason Green, Purdue University, West Lafayette, Indiana, participated in the Interfacial and Condensed-Phase Chemical Physics Summer Research Institute and worked on the study "Soft-Landing of Peptide Ions on Surfaces."

- Yiping Han, State University of New York at Stony Brook, Stony Brook, New York, worked on the study "Development of Data Analysis and Visualization Software – SpectraMiner."

- Hadi Lioe, University of Melbourne, Victoria, Australia, worked on the study "Mechanisms of Fragmentation of Post Translationally Modified Peptides."

- Yong Liu, University of Michigan, Ann Arbor, Michigan, gave the seminar "Aqueous Phase Halogen Free Reactions: $X+X^{-}\leftrightarrow X_2^{-}$ (X=Br, I)."

- Anoop Mayampurath, Utah State University, Logan, Utah, participated in the Interfacial and Condensed-Phase Chemical Physics Summer Research Institute and worked on the study "Develop a Procedure for the Determination of the Calibration Parameters on the

Host Side and Integrate Them into the Hardware to Facilitate Real Time Multiband Analysis."

- Howard Mayne, University of New Hampshire, Durham, New Hampshire, gave the seminar "Exploring the Rugged Landscape: Towards Understanding and Manipulating the Properties of Mixed Atomic van der Waals Clusters."

- Vladimir Mikheev, Innovatek, Inc., Richland, Washington, worked on the ongoing research collaboration "Ultra-Trace Molecular Detection Instrumentation Based on Aerosol Nucleation with Rapid Preconcentration and Separation."

- Bill Robertson, University of California, Irvine, California, worked on the study "Laboratory Studies of Atmospheric Processing of Sea Salt."

- Luis Rodriguez, National Cancer Institute, Bethesda, Maryland, worked on the study "Development of Multi-Functional Microscopy (MFM) for Cancer and AIDS Research."

- Andy Shaller, Washington State University, Pullman, Washington, participated in the Interfacial and Condensed-Phase Chemical Physics Summer Research Institute and worked on the study "Single Molecule Dynamics of Protein DNA Interactions."

- Tieqiao Zhang, National Institutes of Health, Bethesda, Maryland, worked on the study "Analysis of Lipid Nanoparticle Interaction with Cell Membrane."

- Zhenrong Zhang, University of Texas at Austin, Texas, participated in the Interfacial and Condensed-Phase Chemical Physics Summer Research Institute and worked on the study "Photochemistry of Halogenated Hydrocarbon on TiO_2(110) Surface."

Environmental Spectroscopy and Biogeochemistry Facility

- Andrew Del Negro and Zheming Wang, Pacific Northwest National Laboratory, Richland, Washington, measured the luminescence and excited-state lifetime properties of the newly discovered Tc(V) chromophore. This project features a collaboration with researchers from the University of Cincinnati (CJ Seliskar and WR Heineman), University of Wyoming (BP Sullivan), and Pacific Northwest National Laboratory (TL Hubler and SA Byran) and involves the spectroelectrochemical detection of pertechnetate in the vadose zone. The Tc(V) complexes studied here are the first examples of luminescent technetium complexes. Measurements to determine quantum yield and absorption spectral data as well as detailed studies of the temperature dependence of the photophysical properties of the technetium complexes are currently underway.

- Baolin Deng, University of Missouri-Columbia, Columbia, Missouri, along with Chongxuan Liu and Eugene Ilton, Pacific Northwest National Laboratory, Richland, Washington, continued their collaboration using X-ray photoelectron spectroscopy and surface complexation modeling to investigate Cr(VI) removal from waste water by a quanternized polymer coated activated carbon.

- Erica DiFilippo (Figure 18), a graduate student from the laboratory of Mark Brusseau at the University of Arizona, Tucson, Arizona, is working with scientists Mart Oostrom, Pacific Northwest National Laboratory, Richland, Washington, and EMSL researcher Tom Wietsma to investigate the amount of dense nonaqueous phase liquid mass flux reduction as a function of source zone mass removal. This relationship will be useful in evaluating the benefit of partial source zone mass removal.

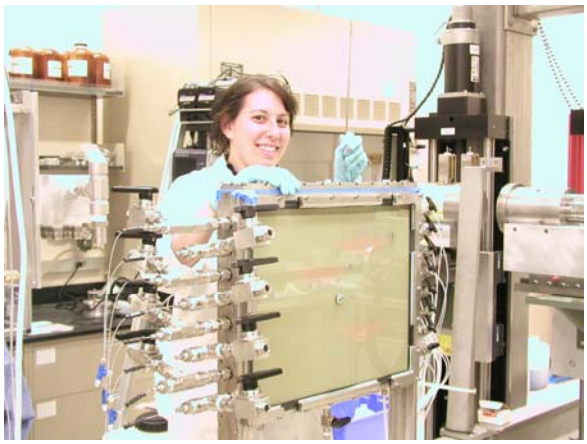

Figure 18. Erica DiFilippo

- Carrick Eggleston (Figure 19), University of Wyoming, Laramie, Wyoming, is working with Kevin Rosso and Brian Lower, Pacific Northwest National Laboratory, Richland, Washington, to examine the electron-transfer properties of outer-membrane cytochromes from the metal-reducing bacterium *Shewanella oneidensis*. As part of EMSL's Biogeochemistry Scientific Grand Challenge, the overall goal of this work is to examine how certain proteins control electron transfer between iron-reducing bacteria and ferric minerals.

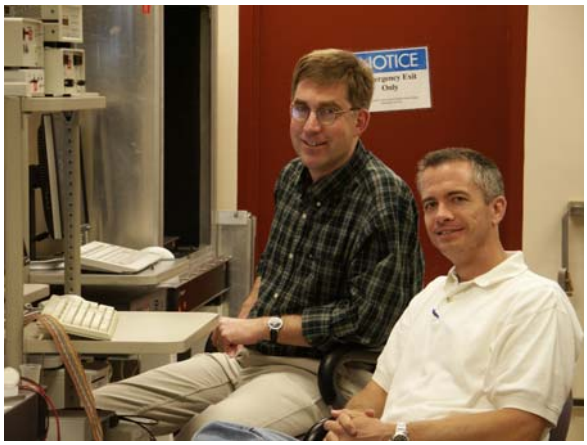

Figure 19. Carrick Eggleston and Kevin Rosso

- Daniel Ewert, John Adamec, and Meg Pinza, Pacific Northwest National Laboratory, Sequim, Washington, and Zheming Wang, Pacific Northwest National Laboratory, Richland, Washington, continued measuring the fluorescence spectra of fungi samples grown under different aqueous conditions. Fungi may have the potential to be developed as novel marine biosensors and enhanced biosentinels to detect biological weapons in marine systems.

- Leila Reynald, Johns Hopkins University, Baltimore, Maryland, and EMSL researcher Paul Gassman continued to evaluate the effect of mutation in the *Staphylococcal* nuclease protein on water structure within the hydrophobic core using room-temperature and

cryogenic Fourier-transform infrared microscopy. Abnormal structures of other proteins may be responsible for diseases such as Alzheimer's disease, cystic fibrosis, bovine spongiform encephalopathy (Mad Cow disease), and even many cancers.

- Frannie Skomurski (Figure 20), University of Michigan, Ann Arbor, Michigan, is working with Kevin Rosso, Pacific Northwest National Laboratory, Richland, Washington, to investigate the interaction between uranium in solution and mineral magnetite (Fe_3O_4). Computer modeling is used to simulate the adsorption of aqueous U^{6+} onto different magnetite surfaces, and electron transfer calculations are performed to understand the process of reduction, and hence immobilization, of U^{6+} by Fe^{2+}. Complementary adsorption experiments are performed using atomic force and scanning tunneling microscopy on natural magnetite samples, as well as on epitaxially grown magnetite thin films from PNNL. This research relates to understanding the role of iron-oxides in immobilizing uranium in the environment, and is supported by the DOE Office of Civilian and Radioactive Waste Management's student fellowship program.

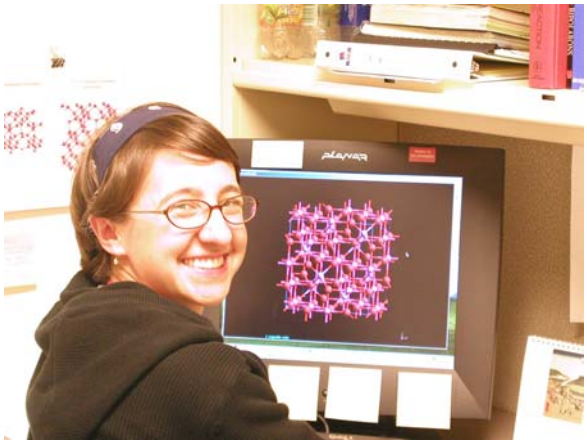

Figure 20. Frannie Skomurski

- Matthew Wander (Figure 21), a graduate student from the laboratory of Martin Schoonen at Stony Brook University, Stony Brook, New York, is working with Kevin Rosso, Pacific Northwest National Laboratory, Richland, Washington, to study homogeneous and heterogeneous redox processes in aqueous systems. First, they are to examine the effects of pH and carbonate on uranium reduction kinetics by iron. Second, they are beginning characterization of the reductive potential of green rust and its ability to reduce chromate pollution.

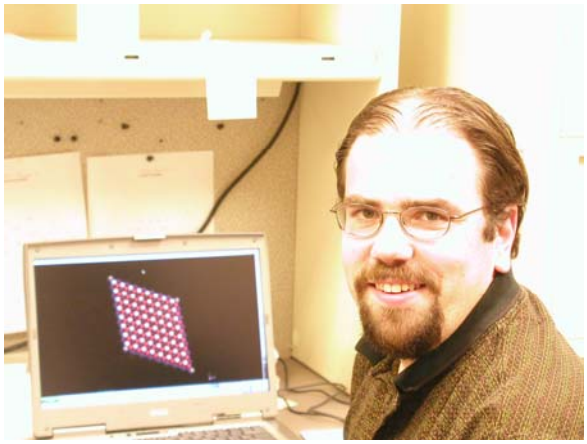

Figure 21. Matthew Wander

- John H. Weare, on sabbatical from the University of California, San Diego, La Jolla, California, visited EMSL to continue his collaboration with Eric J. Bylaska, Pacific Northwest National Laboratory, Richland, Washington, and EMSL researcher Marat Valiev. They are studying high-temperature (pressure) electrolyte solutions thought to

facilitate metal ion transport in hydrothermal environments by using *ab initio* molecular dynamics methods, which require a parallel computational environment such as that provided by the EMSL supercomputer.

High-Field Magnetic Resonance Facility

- Geoffrey Bowers, Pennsylvania State University, University Park, Pennsylvania, recently used the 900-MHz spectrometer onsite for the study "Sensitivity Enhancing NMR of Strontium-87 Nuclei in Environmental Samples."

- Peter Brzovic and Ponni Rajagopal, University of Washington, Seattle, Washington, worked remotely on the 900-MHz spectrometer for the study "NMR Structural Investigations of BRCA1."

- Leonard Fifield, Pacific Northwest National Laboratory, Richland, Washington, used the 300-MHz and 500-MHz spectrometers onsite for the study "NMR Analysis of Synthesized Organic Compounds for Modification of Nanostructures."

- Jian Zhi Hu, Pacific Northwest National Laboratory, Richland, Washington, used the 900-MHz spectrometer onsite for "*In-situ* High Field, High Field NMR Spectrometry."

- Doug Klewer, Arizona State University, Tempe, Arizona, used the 800-MHz spectrometer onsite for the study "Structure and Function of the Membrane Protein OEP16."

- Thomas Leeper, University of Washington, Seattle, Washington, worked remotely on the 600-MHz spectrometer for the study "Structure of Telomerase RNA."

- Andrew Lipton, Pacific Northwest National Laboratory, Richland, Washington, used the 900-MHz and 800-MHz spectrometers onsite for the studies "Correlation of Structure and Function of Zinc Metalloproteins via Solid-State NMR Methods" and "Investigation of the Role of Mg^{2+} in DNA Repair Proteins APE1, Pol, and FEN1."

- Raymond Reeves, Washington State University, Pullman, Washington, used the 900-MHz, 800-MHz, 600-MHz, 750-MHz, and 500-MHz spectrometers onsite for the study "Structural Biology of the Human High Mobility Group A (HMGA) Proteins."

- Celine Schneider and Franziska Scheffler, University of British Columbia, Vancouver, British Columbia, Canada, used the 800-MHz spectrometer onsite for the study "Structural Investigations of Solid Materials by High Resolution Solid State NMR at Very High Field."

- Wendy Shaw, Pacific Northwest National Laboratory, Richland, Washington, used the 500-MHz spectrometer onsite for the study "Hydrogen Storage Materials."

- Thomas Squier, Pacific Northwest National Laboratory, Richland, Washington, used the 500-MHz spectrometer onsite for the study "Development of Multi Purpose Tags and Affinity Reagents or Rapid Isolation and Visualization of Protein Complexes."

- Weixing Xu, University of Central Florida, Orlando, Florida, recently used the 300-MHz spectrometer onsite for "Study of the Network Structures of Polymer-Derived Amorphous SiAlCN Ceramics."

- Gary Yang, Pacific Northwest National Laboratory, Richland, Washington, used the 300-MHz spectrometer onsite for the study "NMR Study of Effects and Mechanisms of Mechanical Activation on Hydrogen Sorption/Desorption of Nanoscale Lithium Nitrides."

The following individuals sent samples to be run on the 900-MHz, 750-MHz, and 600-MHz cryoprobe NMR spectrometers in support of EMSL's Structural Genomics Collaborative Access Team, led by Michael Kennedy, Pacific Northwest National Laboratory, Richland, Washington:

- Cheryl Arrowsmith, University of Toronto, Toronto, Ontario, Canada

- Guy Montelione, Rutgers University, Piscataway, New Jersey

- Tom Terwilliger, Los Alamos National Laboratory, Los Alamos, New Mexico.

High-Performance Mass Spectrometry Facility

- Josh Adkins, Pacific Northwest National Laboratory, Richland, Washington, worked on the study "Identifying Targets for Therapeutic Interventions using Proteomic Technology." Significant progress has been made towards identifying key proteins that attribute to the pathogenicity of *Salmonella typhimurium in vivo* and *in vitro*. A mass tag database has been built for this organism, and progress is being made on other organisms involved in this study.

- Joel A. Klappenbach, Michigan State University, East Lansing, Michigan, worked on the study "Intra-Species Proteome within a Natural Population of *Shewanella baltica*." Thirteen strains of *Shewanella baltica* were received at EMSL and processed with the intent of building mass tag databases for each strain. The samples are currently being analyzed by liquid chromatography and liquid chromatography-tandem mass spectrometry, with data analysis to follow.

- Tao Liu, Pacific Northwest National Laboratory, Richland, Washington, worked on the study "Global Analysis of the Response of Human Mammary Epithelial Cells (HMEC) to Epidermal Growth Factor (EGF) Stimulation." The AMT databases for cysteinyl- and global tryptic peptides from both HMEC cell lysates and secreted proteins have been populated, with 6,518 nonredundant proteins identified. Time-course studies of EGF-stimulated HMEC samples (0, 0.25, 1, 4, 8, 13, 18, and 24 hours) have been conducted using the quantitative cysteinyl-peptide enrichment technology approach, with 2,243 proteins quantified (from $^{18}O/^{16}O$-labeled peptides), and among them more than 500 proteins were found significantly changed in abundance. Collaborators from PNNL's Cell Biology Group are integrating data from microarray, parallel Western blot, and proteomic studies, and a manuscript is currently in progress.

- Derek Lovley and his research group, University of Massachusetts, Amherst, Massachusetts, are collaborating with EMSL researcher Kim Hixson on the study "Global Proteomic Analysis of *Geobacter sulfurreducens*." A manuscript was submitted to the *Journal of Bacteriology* that shows the side-by-side protein abundance comparison of 3,300 proteins expressed by *Geobacter sulfurreducens* under eight different environmentally relevant growth conditions. Additionally, predominant protein sub-cellular location of 91 c-type cytochromes was determined by comparing protein abundances of sucrose gradient centrifugation separated fractions of inner, outer, and periplasm proteins in culture conditions using either ferric citrate or fumarate as the end electron acceptor.

- Donald Moerman, University of British Columbia, Vancouver, Canada, worked on the study "A Proteome for Specific Cell Types in *Caenorhabditis Elegans*." Moerman is investigating protein expression patterns in the 550 cell whole embryo and isolated FAC sorted myo-3::GFP labeled muscle cells, using a combination of enzymatic digestion, high-resolution liquid chromatography-Fourier transform ion cyclotron resonance (FTICR) mass spectrometry and the accurate mass and time (AMT) tag strategy to build a snapshot of the proteome in these two samples. More than 1,000 muscle proteins were identified by searching the FTICR data in the AMT tag database. In addition, he was able to identify a large number of predicted and partially confirmed proteins from both embryos and muscle cells.

- Liang Shi, Pacific Northwest National Laboratory, Richland, Washington, worked on the study "Unraveling the Molecular Biology of Host-Pathogen Interactions." Shi has submitted several trial samples to determine the best method for isolating *Salmonella*-containing vacuoles (SCV) in macrophage cells. They have been processed and are currently in the queue for instrumental analysis. As soon as the appropriate method is identified, further proteomic studies will be performed to elucidate the mechanisms behind SCV.

Interfacial and Nanoscale Science Facility

- Pulickel Ajayan, Rensselaer Polytechnic Institute, Troy, New York, gave the seminar "Controlled Fabrication of Carbon Nanotube Architectures." He also explored the possibilities for collaborations using the accelerator facility to characterize samples.

- Zsuzsanna Balogh, Washington State University, Pullman, Washington, used the electron microscopy suite to characterize mineral nanostructures in order to understand issues associated with soil mineral weathering.

- Joe Cecil, New Mexico State University, Las Cruces, New Mexico, participated in meetings with EMSL staff to learn about Interfacial and Nanoscale Science Facility capabilities for possible future collaborations.

- Anthony Cinson, Wheeling Jesuit University, Wheeling, West Virginia, visited EMSL as part of a Department of Homeland Security Fellowship to study the influence of

gadolinium and samarium doping on atomic and ionic transport properties of novel nanostructured ceria-zirconia multilayers.

- Mike Dyer, Florida State University, Tallahassee, Florida, visited EMSL as a part of the Summer Research Institute to investigate the effects of strain and stress due to lattice mismatch in thin film zirconia on yttria-stabilized zirconia substrates.

- Shiho Iwanaga, University of Washington, Seattle, Washington, carried out fundamental research in synthesis and characterization of thermoelectric materials.

- Satya Kuchibhatla from the University of Central Florida, Orlando, Florida, visited EMSL as a part of the Summer Research Institute to investigate the properties of free-standing ceria nanoparticles and ceria nanodomains in thin films.

- Justin Nairn, University of Idaho, Moscow, Idaho, recently used the high-resolution transmission electron microscope to image nanoparticles in order to understand the effect of photolysis time, solvent, different passivating agents, and annealing on their size and size distribution.

- Fung Suong Ou, Rensselaer Polytechnic Institute, Troy, New York, visited EMSL as part of the Summer Research Institute to conduct research on controlled defect generation in porous silicon.

- Lea Ream, Yakima Valley Community College, Yakima, Washington, visited EMSL as a part of the community college initiative to investigate surface modification by high-energy ion beams.

- Yiguang Wang, University of Central Florida, Orlando, Florida, visited EMSL as a part of the Summer Research Institute to synthesize oxide electrolyte layer-by-layer structures using sputter deposition capabilities and characterize these films using various capabilities.

- Atsushi Yamamoto, Energy Technology Research Institute, Ibaraki, Japan, carried out fundamental research in synthesis and characterization of thermoelectric materials.

Molecular Science Computing Facility, Visualization and User Services Group

- Kenley Barrett (Figure 22), a graduate student from Northwestern University, Evanston, Illinois, visited EMSL to learn how to effectively use both Ecce and NWChem. She is part of EMSL's Computational Grand Challenge project "Direct Dynamics Simulations: From Molecules to Macromolecules and Condensed Phases," now in its second year.

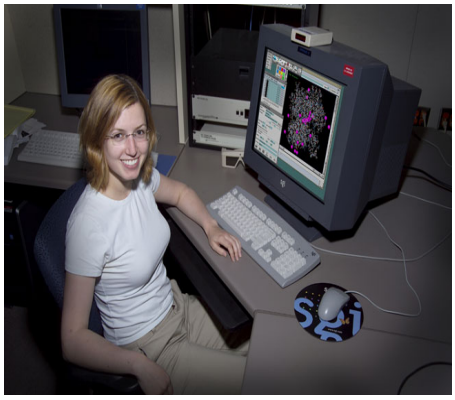

Figure 22. Kenley Barrett from Northwestern University. Barrett is using Ecce in EMSL's Graphics and Visualization Laboratory to visualize the protein complex actin.

Molecular Science Computing Facility, Molecular Science Software Group

- Adam Mickiewicz University, Poznan, Poland
- Boston College, Chestnut Hill, Massachusetts
- Cankaya University, Ankara, Turkey
- COSMOlogic, Leverkusen, Germany
- Delta Search Labs, Cambridge, Massachusetts
- Eotvos University, Budapest, Hungary
- Fujitsu Limited, Chiba, Japan
- German Cancer Research Center, Heidelberg, Germany
- Hokkaido University, Center for Advanced Research of Energy, Sapporo, Japan
- A.V. Palladin Institute of Biochemistry of the Ukrainian National Academy, Kiev, Ukraine
- John Jay College-City University of New York, New York
- Korea Institute of Science and Technology, Seoul, South Korea
- Kutztown University, Kutztown, Pennsylvania

- Mississippi State University, Mississippi State, Mississippi
- Moscow State University, Moscow, Russia
- North Carolina A & T State University, Greensboro, North Carolina
- Purdue University, West Lafayette, Indiana
- Rhodes College, Memphis, Tennessee
- Samara State Technical University, Samara, Russia
- Shanghai Supercomputer Center, Shanghai, China
- Swiss Federal Institute of Technology, Zurich, Switzerland
- Texas A&M University, College Station, Texas
- T-Graphic, Littleton, Colorado
- Universidad Autonoma Metropolitana, Iztapalapa, Mexico
- University of Chicago, Chicago, Illinois
- University of Chile, Santiago, Chile
- University of Cincinnati, Cincinnati, Ohio
- University of Coimbra, Coimbra, Portugal
- University of Copenhagen, Copenhagen, Denmark
- University of Hannover, Hannover, Germany
- University of Maryland, College Park, Maryland
- University of Milano, Milan, Italy
- University of Nevada, Las Vegas, Nevada
- University of North Carolina, Renaissance Computing Institute, Chapel Hill, North Carolina
- University of Oklahoma, Norman, Oklahoma
- University of Oxford, Oxford, United Kingdom

- University of Padova, Padova, Italy
- University of Richmond, Richmond, Virginia
- University of Sao Paulo, Sao Carlos, Brazil
- University of Siena, Siena, Italy
- University of Tennessee, Knoxville, Tennessee
- University of the Pacific, Stockton, California
- University of Toronto, Toronto, Ontario, Canada
- University of Ulm, Ulm, Germany
- University of Washington, Seattle, Washington
- Virginia Polytechnic Institute, Terascale Computing Facility, Blacksburg, Virginia
- Washington State University, Pullman, Washington
- Westfaelische Wilhelms Universitaet, Muenster, Germany
- York College-City University of New York, Jamaica, New York

New EMSL Staff

None

Publications

The following list represents publications by EMSL staff members and users where the publication resulted from research carried out at EMSL.

Alvarez J, RG Cooks, SE Barlow, DJ Gaspar, JH Futrell, and J Laskin. 2005. "Preparation and *in situ* Characterization of Surfaces Using Soft Landing in a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer." *Analytical Chemistry* 77(11):3452-3460.

Azad S, MH Engelhard, and LQ Wang. 2005. "Adsorption and Reaction of CO and CO_2 on Oxidized and Reduced $SrTiO_3$ (100) Surfaces." *Journal of Physical Chemistry B* 109(20):10327-10331.

Chen L, WA de Jong, and J Ye. 2005. "Characterization of the Molecular Iodine Electronic Wave Functions and Potential Energy Curves through Hyperfine Interactions in the $B0u^+$ (^{3}IIu) State." *Journal of the Optical Society of America B* 22(5):951-961.

Chen W, S Wang, SL Westcott, J Zhang, K Dou, AG Joly, and DE McCready. 2005. "Structure and Luminescence of BaFBr:Eu^{2+} and BaFBr:Eu^{2+}, Tb^{3+} Phosphors and Thin Films." *Journal of Applied Physics* 97(8):083506 (pages 1 - 8).

Daschbach JL, Z Dohnalek, SR Liu, RS Smith, and BD Kay. 2005. "Water Adsorption, Desorption, and Clustering on FeO(111)." *Journal of Physical Chemistry B* 109(20):10362-10370.

DeYonker,NJ, S Li, Y Yamaguchi, HF Schaefer III, TD Crawford, RA King, and KA Peterson. 2005. "Application of Equation-of-Motion Coupled-Cluster Methods to Low-Lying Singlet and Triplet Electronic States of HBO and BOH." *Journal of Chemical Physics* 122(23):234316, 1–13.

Douglas M, SB Clark, JI Friese, BW Arey, EC Buck, and BD Hanson. 2005. "Neptunium(V) Partitioning to Uranium(VI) Oxide and Peroxide Solids." *Environmental Science and Technology* 39(11):4117-4124.

Gao F, EJ Bylaska, and WJ Weber. 2005. "Defect Properties in GaN: *ab initio* and Empirical Potential Calculations." *Materials Science Forum* 475-479(1-5):3087-3090.

Griffin KA, AB Pakhomov, CM Wang, SM Heald, and KM Krishnan. 2005. "Cobalt-Doped Anatase TiO_2: A Room Temperature Dilute Magnetic Dielectric Material." *Journal of Applied Physics* 97(10):10D320 (pages 1 – 3).

Gutierrez F, C Rabbe, R Poteau, and JP Daudey. 2005. "Theoretical Study of Ln(III) Complexes with Polyaza-Aromatic Ligands: Geometries of $[LnL(H_2O)_n]^{3+}$ Complexes and Successes and Failures of TD-DFT." *Journal of Physical Chemistry A* 109(19):4325-4330.

Gutowska A, L Li, Y Shin, CM Wang, XS Li, JC Linehan, RS Smith, BD Kay, B Schmid, W Shaw, M Gutowski, and T Autrey. 2005. "Nanoscaffold Mediates Hydrogen Release and the Reactivity of Ammonia Borane." *Angewandte Chemie International Edition* 44(23):3578-3582.

Havre SL, M Singhal, DA Payne, MS Weir Lipton, and BJM Webb-Robertson. 2005. "Enabling Proteomics Discovery through Visual Analysis." *IEEE Engineering in Medicine and Biology* 24(3):50-57.

Hu DH, and HP Lu. 2005. "Single-Molecule Triplet-State Photon Antibunching at Room Temperature." *Journal of Physical Chemistry B* 109(20):9861-9864.

Iordanova N, M Dupuis, and KM Rosso. 2005. "Charge Transport in Metal Oxides: A Theoretical Study of Hematite α-Fe_2O_3." *Journal of Chemical Physics* 122(14):144305 (pages 1 – 10).

Johnson MC, Z Liliental-Weber, DN Zakharov, DE McCready, RJ Jorgensen, J Wu, W Shan, and ED Bourret-Courchesne. 2005. "Investigation of Microstructure and V-Defect Formation in In_xGa_1-xN/GaN MQW Grown using Temperature-Gradient Metalorganic Chemical Vapor Deposition." *Journal of Electronic Materials* 34(5):605-611.

Joly AG, W Chen, DE McCready, JO Malm, and JO Bovin. 2005. "Upconversion Luminescence of CdTe Nanoparticles." *Physical Review B* 71(16):165304 (pages 1 - 9).

Kim S, SE Wheeler, NJ Deyonker, and HF Schaefer III. 2005. "The Extremely Flat Torsional Potential Energy Surface of Oxalyl Chloride." *Journal of Chemical Physics* 122(23):234313, 1-4.

Laskin A, TW Wietsma, BJ Krueger, and VH Grassian. 2005. "Heterogeneous Chemistry of Individual Mineral Dust Particles with Nitric Acid: A Combined CCSEM/EDX, ESEM, and ICP-MS Study." *Journal of Geophysical Research* 110:D10208 (pages 1 - 15).

Lee K, S Jockusch, NJ Turro, RH French, RC Wheland, MF Lemon, AM Braun, T Widerschpan, DA Dixon, J Li, M Ivan, and P Zimmerman. 2005. "157 nm Pellicles (Thin Films) for Photolithography: Mechanistic Investigation of the VUV and UV-C Photolysis of Fluorocarbons." *Journal of the American Chemical Society* 127(23):8320-8327.

Lee M, H Kim, YS Lee, and MS Kim. 2005. "A Dramatic Spin-Orbit Effect Observed in the Vibrational Frequencies of the Chloroiodomethane Cation." *Angewandte Chemie* 117(19):2989-2991.

Li X, B Kiran, and LS Wang. 2005. "Gold as Hydrogen. An Experimental and Theoretical Study of the Structures and Bonding in Disilicon Gold Clusters $Si_2Au_n^-$ and Si_2Au_n (n=2 and 4) and Comparisons to Si_2H_2 and Si_2H_4." *Journal of Physical Chemistry A* 109(19):4366-4374.

Osterwalder J, T Droubay, T Kaspar, J Williams, CM Wang, and SA Chambers. 2005. "Growth of Cr-doped TiO_2 Films in the Rutile and Anatase Structure by Oxygen Plasma Assisted Molecular Beam Epitaxy." *Thin Solid Films* 484(1-2):289-298.

Qian WJ, ME Monroe, T Liu, JM Jacobs, GA Anderson, Y Shen, RJ Moore, DJ Anderson, R Zhang, SE Calvano, SF Lowry, W Xiao, LL Moldawer, RW Davis, RG Tompkins, DG Camp, II, RD Smith, and the Inflammation and the Host Response to Injury Large Scale Collaborative Research Program. 2005. "Quantitative Proteome Analysis of Human Plasma Following *in vivo* Lipopolysaccharide Administration using $^{16}O/^{18}O$ Labeling and the Accurate Mass and Time Tag Approach." *Molecular & Cellular Proteomics* 4(5):700-709.

Ramirez-Solis A, R Poteau, A Vela, and JP Daudey. 2005. "Comparative Studies of the Spectroscopy of $CuCl_2$: DFT Versus Standard *Ab Initio* Approaches." *Journal of Chemical Physics* 122(16):164306, 1-10.

Roberts BK, AB Pakhomov, VS Shutthanandan, and KM Krishnan. 2005. "Ferromagnetic Cr-doped ZnO for Spin Electronics via Magnetron Sputtering." *Journal of Applied Physics* 97(10):10D310 (pages 1 – 3).

Rosso KM, and ES Ilton. 2005. "Effects of Compositional Defects on Small Polaron Hopping in Micas." *Journal of Chemical Physic*s 122(24):244709, 1-9.

Sani RK, BM Peyton, A Dohnalkova, and JE Amonette. 2005. "Reoxidation of Reduced Uranium with Iron(III) (Hydr)Oxides under Sulfate-Reducing Conditions." *Environmental Science and Technology* 39(7):2059-2066.

Saraf L, DR Baer, Z Wang, J Young, MH Engelhard, and S Thevuthasan. 2005. "Hydrogen Bubbles and Formation of Nanoporous Silicon during Electrochemical Etching." *Surface and Interface Analysis* 37(6):555-561.

Saraf L, CM Wang, V Shutthanandan, Y Zhang, O Marina, DR Baer, S Thevuthasan, P Nachimuthu, and DW Lindle. 2005. "Oxygen Transport Studies in Nanocrystalline Ceria Films." *Journal of Materials Research* 20(5):1295-1299.

Shakya SK, W Gu, and V Helms. 2005. "Molecular Dynamics Simulation of Truncated Bovine Adrenodoxin." *Biopolymers* 78(1):9-20.

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Swaddle TW, J Rosenqvist, P Yu, E Bylaska, BL Phillips, and WH Casey. 2005. "Kinetic Evidence for Five-Coordination in $AlOH(aq)^{2+}$ Ion." *Science* 308(5727):1450-1453.

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Tait SL, Z Dohnalek, CT Campbell, and BD Kay. 2005. "*n*-Alkanes on MgO(100). II. Chain Length Dependence of Kinetic Desorption Parameters for Small *n*-Alkanes." *Journal of Chemical Physics* 122(16):164708 (pages 1 - 13).

Tang K, AA Shvartsburg, HN Lee, DC Prior, MA Buschbach, F Li, AV Tolmachev, GA Anderson, and RD Smith. 2005. "High-Sensitivity Ion Mobility Spectrometry/Mass Spectrometry Using Electrodynamic Ion Funnel Interfaces." *Analytical Chemistry* 77(10):3330-3339.

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Zheng F, DN Tran, BJ Busche, GE Fryxell, RS Addleman, TS Zemanian, and CL Aardahl. 2005. "Ethylenediamine-Modified SBA-15 as Regenerable CO_2 Sorbent." *Industrial and Engineering Chemistry Research* 44(9):3099-3105.

Presentations

The following list represents presentations by EMSL staff members and users where the presentations resulted from research carried out at EMSL.

Adkins JN, AD Norbeck, HM Mottaz, T Clauss, J Gustin, J Rue, F Heffron, and RD Smith. 2005. "Proteomics as a Tool for Identifying Targets for Therapeutic Interventions of Possible BioTerror Agents." Presented by Joshua N. Adkins (Invited Speaker) at the EMSL Review Breakout Session, Richland, Washington, on May 18, 2005.

Adkins JN, AD Norbeck, SO Purvine, J Rue, HM Mottaz, J Gustin, T Clauss, S Wong, F Heffron, and RD Smith. 2005. "Proteomic Identification of Targets for Therapeutic Interventions." Presented by Angela Norbeck (Invited Speaker) at the Microbial Pathogenesis Workshop, Richland, Washington, on May 13, 2005.

Adkins JN, J Rue, HM Mottaz, AD Norbeck, T Clauss, F Heffron, and RD Smith. 2005. "Proteomic Analysis of the Pathogen *Salmonella typhimurium* Under Culture Conditions that Mimic Different Life-Cycle States." Presented by Joshua N. Adkins at the 53rd American Society for Mass Spectrometry Conference, San Antonio, Texas, on June 7, 2005.

Amonette JE, J Kim, CT Garten, Jr, CC Trettin, RS Arvidson, and A Luttge. 2005. "Enhancing Soil Humification: Laboratory Studies with a Model System." Presented by Jim Amonette at the Fourth Annual Conference on Carbon Capture and Sequestration, Alexandria, Virginia, on May 4, 2005.

Amonette JE, V Sarathy, JC Linehan, DW Matson, CM Wang, JT Nurmi, KH Pecher, RL Penn, PG Tratnyek, and DR Baer. 2005. "Chemistry of Metallic Iron Nanoparticles." Presented by James E. Amonette at the 15th Annual V. I. Goldschmidt Conference, Moscow, Idaho, on May 21, 2005.

Ayotte P, JL Daschbach, Z Dohnalek, GA Kimmel, KP Stevenson, GR Teeter, RS Smith, and BD Kay. 2005. "Using Nanoscale Amorphous Films to Study Processes in Supercooled Liquid Water and Aqueous Solutions." Presented by Bruce Kay (Invited Speaker) at the International Advisory Board for the Academica Sinica Institute for Atomic and Molecular Sciences, Taipei, Taiwan, Province of China, on June 15, 2005.

Baxter DJ, WR Cannon, and EJ Felix. 2005. "Performance Results for an Application Using LUSTRE as a Shared Global Resource." Presented by Douglas Baxter (Invited Speaker) at the May 2005 Gelato Federation Meeting, San Jose, California, on May 23, 2005.

Beck KM, M Henyk, AG Joly, and WP Hess. 2005. "Comparison of Bulk and Surface Energetics in Metal Oxide Films." Presented by Ken Beck (Invited Speaker) at the annual meeting of the European Commission COST D19/005/01 working group "Chemical Reactivity of Metal Oxide Nanostructures," Torino, Italy, on May 13, 2005.

Bondarchuk O, Z Dohnalek, BD Kay, J Kim, and M White. 2005. "Structure and Catalytic Activity of WO3 Clusters on TiO_2(110)." Presented by Zdenek Dohnalek (Invited Speaker) at the Department of Energy's Basic Energy Sciences Contractors' Meeting, Rockville, Maryland, on May 19, 2005.

Bruce JE, GA Anderson, N Tolic, X Tang, DP Adhikari, GR Munske, and SM Chowdhury. 2005. "Accurate Mass and PIRs: A New Strategy for Protein Interactions." Presented by James E. Bruce at the 53rd American Society for Mass Spectrometry Conference, San Antonio, Texas, on June 8, 2005

Bruckner-Lea CJ, JN Adkins, ML Alexander, NC Anheier, Jr., CR Batishko, VL Bailey, BP Dockendorff, HC Edberg, SJ Fansler, JW Grate, SA Gray, KK Hixson, KH Jarman, TJ Johnson, MS Lipton, MM Matzke, GP Morgen, SL Owsley, RM Ozanich, GJ Posakony, TM Straub, KL Wahl, NB Valentine, CO Valdez, P Valdez, CL Warner, and MG Warner. 2005. "Next Generation Bioassays and Biodetection Systems for Homeland Security." Presented by Cindy Bruckner-Lea at the Homeland Security Advance Research Projects Agency Bioinformatics and Assays Development Program/Bioagents Autonomous Networked Detector Conference, Pleasanton, California, on May 11, 2005.

Bylaska EJ, and GD Black. 2005. "NWChem and ECCE Training at ARL." Presented by Eric Bylaska (Invited Speaker) at NWChem and ECCE Training at the U.S. Army Research Laboratory Major Shared Resource Center, Aberdeen, Maryland, on May 9, 2005.

Bylaska EJ, K Tsemekhman, ES Ilton, and KM Rosso. 2005. "Self-Consistent Self-Interaction Corrected DFT Studies of Annite." Presented by Eric Bylaska (Invited Speaker) at the 15th Annual V.I. Goldschmidt Conference, Moscow, Idaho, on May 22, 2005.

Callister SJ, JN Adkins, ME Monroe, CD Goddard, GA Anderson, RD Smith, JK Fredrickson, and MS Lipton. 2005. "Characterization of *Rhodobacter sphaeroides* Aerobic and Photosynthetic Cultures by High Resolution Proteomic Measurements." Presented by Stephen J. Callister at the 53rd American Society for Mass Spectrometry Conference, San Antonio, Texas, on June 8, 2005.

Cannon WR, KH Jarman, BM Webb-Robertson, DJ Baxter, CS Oehmen, KD Jarman, A Heredia-Langner, KJ Auberry, and GA Anderson. 2005. "A Composite Statistical Framework for Peptide Identification from Tandem Mass Spectrometry Data." Presented by William Cannon at the Intelligent Systems in Molecular Biology Conference, Detroit, Michigan, on June 27, 2005.

Casey WH, J Rosenquist, P Yu, BL Phillips, EJ Bylaska, and TW Swaddle. 2005. "Kinetic Evidence for Five-Coordination in the $AlOH_{(aq)}^{2+}$ Ion: Implications for the Reactivity and Toxicity of Aluminum(III) in Water." Presented by Thomas W. Swaddle at the 2005 88th Canadian Chemistry Conference, Saskatoon, Saskatchewan, Canada, on May 30, 2005.

Cliff JB, DJ Gaspar, PJ Bottomley, and DD Myrold. 2005. "Microbial C and N Assimilation in Soils and Model Systems as Revealed by ToF-SIMS." Presented by John Cliff (Invited Speaker) at the 15th Annual V.I. Goldschmidt Conference, Moscow, Idaho, on May 23, 2005.

Cowin JP, and MJ Iedema. 2005. "Proton Solvation and Motion in Water Ices and Their Interfaces." Presented by Jim Cowin (Invited Speaker) at the AirUCI (Air University of California, Irvine) Workshop on Ions and Molecules at Aqueous Interfaces, Prague, Czech Republic, on June 27, 2005.

Craig NC, MC Moore, RL Sams, and DC McKean. 2005. "The Last Lap: High-Resolution Infrared Spectroscopy of Butadiene-2.3-$^{13}C_2$." Presented by Norman Craig (Invited Speaker) at Ohio State University, Columbus, Ohio, on June 22, 2005.

Craig NC, and RL Sams. 2005. "High-Resolution Infrared Spectroscopy of Butadiene: Trans and Gauche Rotamers." Presented by Norman Craig (Invited Speaker) at Ohio State University, Columbus, Ohio, on June 23, 2005.

de Jong WA. 2005. "Actinide Chemistry: Interplay of Computational Modeling and Experiment." Presented by Wibe de Jong (Invited Speaker) at the 24th Rare Earth Research Conference, Keystone, Colorado, on June 27, 2005.

Degliumberto L, DS Perry, W Heiserman, R Cook, HD Mettee, RL Sams, and GO Sorensen. 2005. "The Assymetric N-O Stretch Fundamental Band of Nitromethane: Intramolecular Vibrational Relaxation in the Ground Internal Rotor State." Presented by Lou Degliumberto (Invited Speaker) at Ohio State University, Columbus, Ohio, on June 23, 2005.

Devanathan R, WJ Weber, LR Corrales, A Chartier, and C Meis. 2005. "Computer Simulation of Defect Processes in Complex Ceramics." Presented by Ram Devanathan (Invited Speaker) at the DOE Office of Basic Energy Sciences Project Review, Richland, Washington, on May 11, 2005.

Devineni DP, S Stormo, W Kempf, J Schenkel, R Behanan, AS Lea, and DW Galipeau. 2005. "Nanowires for Automobile and Industrial Emission Detection." Presented by David W. Galipeau at the 2005 Nano Science and Technology Institute Nanotechnology Conference and Trade Show, Anaheim, California, on May 10, 2005.

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