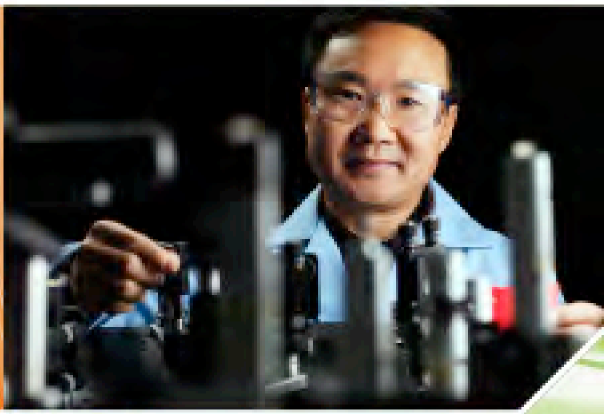
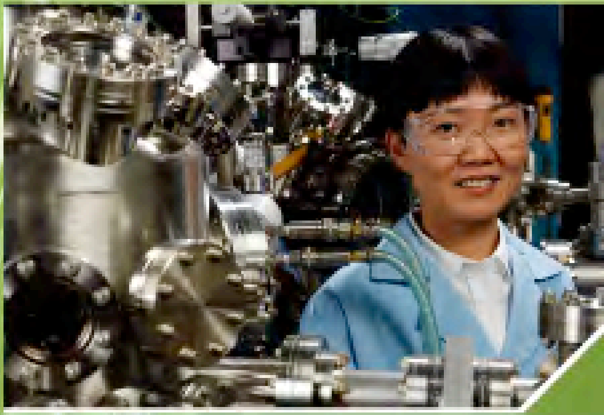
Environmental Molecular
Sciences Laboratory

# EMSL Fiscal Year
# 2008 Annual Report





EMSL

PACIFIC NORTHWEST NATIONAL LABORATORY
*operated by*
BATTELLE
*for the*
UNITED STATES DEPARTMENT OF ENERGY
*under Contract DE-AC05-76RL01830*

**Printed in the United States of America**

**Available to DOE and DOE contractors from the**
**Office of Scientific and Technical Information,**
**P.O. Box 62, Oak Ridge, TN 37831-0062;**
**ph: (865) 576-8401**
**fax: (865) 576-5728**
**email: reports@adonis.osti.gov**

**Available to the public from the National Technical Information Service,**
**U.S. Department of Commerce, 5285 Port Royal Rd., Springfield, VA 22161**
**ph: (800) 553-6847**
**fax: (703) 605-6900**
**email: orders@ntis.fedworld.gov**
**online ordering: http://www.ntis.gov/ordering.htm**

PNNL-18186

# EMSL Fiscal Year 2008 Annual Report

MA Showalter

January 2009

Prepared for the U.S. Department of Energy's Office of Biological and
Environmental Research under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

# Contents

1 Overview ........ 1-1-1

Science Themes ........ 1-1-5

Proposals and Scientific User Access Modes ........ 1-1-5

EMSL Scientific Grand Challenge ........ 1-1-8

EMSL Highlights ........ 1-1-12

Outreach Activities ........ 1-1-36

2-1 Atmospheric Aerosol Chemistry: An Emerging Science Theme ........ 2-1-1

A New Mechanism for Ozonolysis of Unsaturated Organics on Solids: Phosphocholines on NaCl as a Model for Sea Salt Particles ........ 2-1-2
FA Karagulian, AS Lea, and BJ Finlayson-Pitts

Experimental Studies of Heterogeneous Gas-to-Particle Reactions Using Novel Particle-on-Substrate Stagnation Flow Reactor Approach ........ 2-1-4
A Laskin, Y Liu, H Wang, JP Cain, VH Grassian, and ER Gibson

Heterogeneous Reaction of Deliquesced NaCl Particles with Gaseous $HNO_3$ ........ 2-1-6
Y Liu, JP Cain, H Wang, and A Laskin

Laboratory Studies on the Effect of Primary Organic Aerosols on Secondary Organic Aerosol Formation ........ 2-1-8
ML Alexander, C Song, RA Zaveri, JA Thornton, A Zelenyuk, XY Yu, S Madronich, and D Maughan

Application of Methods of High-Resolution Mass Spectrometry to Study Chemistry of Second Organic Aerosol ........ 2-1-11
S Nizkorodov, ML Walser, AP Bateman, A Laskin, J Laskin, and Y Desyaterik

Chemical Speciation of Sulfur in Marine Particles ........ 2-1-12
RJ Hopkins, Y Desyaterik, AV Tivanski, RA Zaveri, CM Berkowitz, T Tyliszczak, MK Gilles, and A Laskin

2-2 Biological Interactions and Dynamics ........ 2-2-1

Submicrometer and Nanoscale Inorganic Particles Exploit the Actin Machinery to be Propelled Along Microvilli into Alveolar Cells ........ 2-2-2
G Orr, DJ Panther, JL Phillips, BJ Tarasevich, A Dohnalkova, D Hu, JG Teeguarden, and JG Pounds

Zinc is Focus of Integrated Studies to Understand Metalloprotein Structure and Function ........ 2-2-5
AS Lipton, RW Heck, M Valiev, WA de Jong, and PD Ellis

Energetics and Dynamics of Electron Transfer and Proton Transfer in Dissociation of Metal$^{III}$(salen)-Peptide Complexes in the Gas Phase ........ 2-2-6
J Laskin, Z Yang, and IK Chu

NMR Bioreactor Development for Live *in situ* Microbial Functional Analysis ........ 2-2-9
PD Majors, JS McLean, and JCM Scholten

The Structure of the GAF A Domain from Phosphodiesterase 6C Reveals Determinants of cGMP-Binding, a Conserved Binding Surface, and a Large cGMP-Dependent Conformational Change........ 2-2-10
SE Martinez, CC Heikaus, RE Klevit, and JA Beavo

Proteomic Characterization of the *Rhodobacter sphaeroides* 2.4.1 Photosynthetic Membrane: Identification of New Proteins ........ 2-2-11
X Zeng, JH Roh, SJ Callister, CL Tavano, TJ Donohue, MS Lipton, and S Kaplan

Making Genomes Accessible: Dealing with the Avalanche of Biological Sequence Data ........ 2-2-13
VM Markowitz

Researchers Utilize Proteomics to Reveal a Core Proteome ........ 2-2-14
SJ Callister, LA McCue, JE Turse, ME Monroe, KJ Auberry, RD Smith, JN Adkins, and MS Lipton

Functional and Structural Characterization of DR_0079 from *Deinococcus radiodurans*, a Novel Nudix Hydrolase with a Preference for Cytosine (Deoxy)Ribonucleoside 5'- Di- and Triphosphates ........ 2-2-16
GW Buchko, O Litvinova, H Robinson, AF Yakunin, and MA Kennedy

Trapped-Ion Cell with Improved DC Potential Harmonicity for FT-ICR MS ........ 2-2-18
AV Tolmachev, EW Robinson, S Wu, H Kang, NM Lourette, L Pasa-Tolic, and RD Smith

Backbone $^{1}H$, $^{13}C$, and $^{15}N$ NMR Assignments for the *Cyanothece 51142* Protein cce_0567: A Protein Associated with Nitrogen Fixation in the DUF683 Family ... 2-2-19
GW Buchko and HJ Sofia

Researchers Integrate Computing and Experiments to Gain Insight in the Structure and Function of Enzymes and Peptides ........ 2-2-20

2-3 Geochemistry/Biogeochemistry and Subsurface Science ........ 2-3-1

Understanding Uranium Complex Formation through Combined Modeling and Gas-Phase Experiments ........ 2-3-2
WA de Jong, GS Groenewald, MJ Van Stipdonk, and L Visscher

Carbon Tetrachloride Flow and Transport in the Subsurface of the 216-Z-9 Trench at the Hanford Site .......... 2-3-4
M Oostrom, ML Rockhold, PD Thorne, MJ Truex, GV Last, and VJ Rohay

Geochemical Controls on Contaminant Uranium in Vadose Hanford Formation Sediments at the 200 Area and 300 Area, Hanford Site, Washington .......... 2-3-6
JP McKinley, JM Zachara, J Wan, DE McCready, and SM Heald

*In vitro* Evolution of a Peptide with a Hematite Binding Motif that May Constitute a Natural Metal-Oxide Binding Archetype .......... 2-3-8
BH Lower, RD Lins, ZW Oestreicher, TP Straatsma, MF Hochella, Jr., L Shi, and SK Lower

2-4 Science of Interfacial Phenomena .......... 2-4-1

Transient Mobility of Oxygen Adatoms upon $O_2$ Dissociation on Reduced $TiO_2(110)$ .......... 2-4-2
Y Du, Z Dohnalek, and IV Lyubinetsky

Probing Reaction Pathways using *in situ* $^1$H NMR Spectroscopy .......... 2-4-3
L Shaw, JZ Hu, JH Kwak, and Z Yang

A Multinuclear MAS NMR Investigation of the Environmentally Relevant Material Magnesium Aluminum Layered Double Hydroxides .......... 2-4-6
JL Palumbo, PJ Sideris, and CP Grey

Nuclear Spin Relaxation of $^{207}$Pb in Ferroelectric Powders .......... 2-4-8
LS Bouchard, AO Sushkov, D Dudker, JJ Ford, and AS Lipton

One Step Closer to Hydrogen-Powered Cars .......... 2-4-10
J Knudson, AU Nilekar, RT Vang, J Schadt, EL Kunkes, JA Dumesic, M Mavrikakis, and F Besenbacher

900-MHz NMR Enables Novel Catalysis Studies .......... 2-4-11
JH Kwak, JZ Hu, DH Kim, J Szanyi, and CHF Peden

Microstructures of ZnO Films Deposited on (0001) and r-cut $\alpha$-$Al_2O_3$ Using Metal Organic Chemical Vapor Deposition .......... 2-4-13
CM Wang, LV Saraf, and Y Qiang

Direct Synthesis of Nanoceria in Aqueous Polyhydroxyl Solutions .......... 2-4-14
AS Karakoti, AS Kuchibhatla, KS Babu, and S Seal

Hidden Ferromagnetic Secondary Phases in Cobalt-Doped ZnO Epitaxial Thin Films .......... 2-4-16
TC Kaspar, T Droubay, SM Heald, MH Engelhard, P Nachimuthu, and SA Chambers

Alcohol Chemistry on Rutile $TiO_2(110)$: The Influence of Alkyl Substituents on Reactivity and Selectivity .......... 2-4-18
YK Kim, BD Kay, JM White, and Z Dohnalek

Conductivity of Oriented Samaria-Doped Ceria Thin Films Grown by Oxygen-Plasma-Assisted Molecular Beam Epitaxy .......... 2-4-21
ZQ Yu, SV Kuchibhatla, LV Saraf, OA Marina, CM Wang, MH Engelhard, V Shutthanandan, P Nachimuthu, and S Thevuthasan

Laser and Electrical Current Induced Phase Transformation of $In_2Se_3$ Semiconductor Thin Film on Si(111) .......... 2-4-23
CY Lu, PJ Shamberger, EN Yitamben, KM Beck, AG Joly, MA Almstead, and FS Ohuchi

A Fast Analysis Technique to Evaluate Scintillation Response .......... 2-4-25
Y Zhang, M Elfman, BD Milbrath, and WJ Weber

Enhanced Understanding of Titania's Catalytic Mechanism through Computational Modeling .......... 2-4-29
S Kerisit, NA Deskins, KM Rosso, and M Dupuis

3 User Projects .......... 3-1-1

4 Publications .......... 4-1-1

# Overview

This Fiscal Year 2008 Annual Report describes the research and accomplishments of staff and scientific users of EMSL—the Environmental Molecular Sciences Laboratory, located in Richland, Washington.

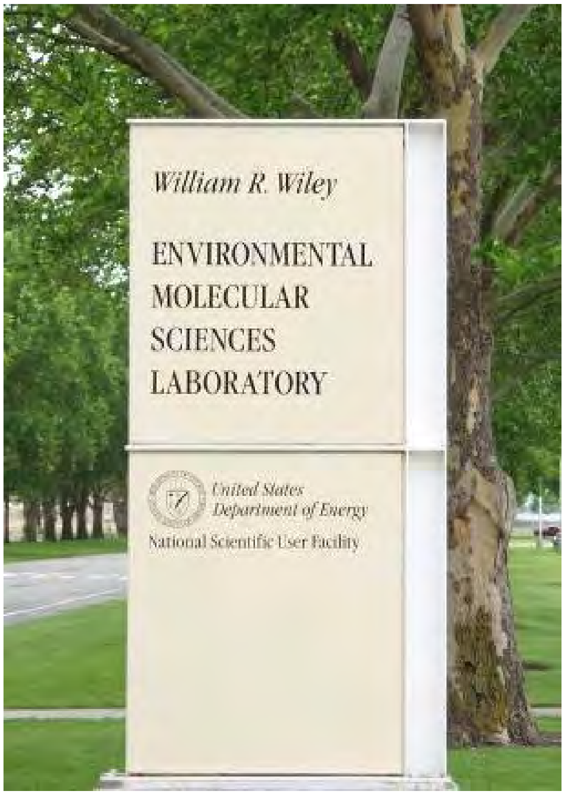
## *Mission*

> *EMSL, a national scientific user facility at Pacific Northwest National Laboratory, provides integrated experimental and computational resources for discovery and technological innovation in the environmental molecular sciences to support the needs of DOE and the nation.*

EMSL strives for simultaneous excellence in 1) high-impact science and marquee capabilities, 2) outstanding management and operations, and 3) exceptional user outreach and services, and uses these tenets to deliver its mission and implement its strategy. The central focus of EMSL's strategy is delivery on the mission of the scientific user facility. In addition to its mission, EMSL has a vision and strategy that show where the scientific user facility intends to be in the next 10 years and the progress that will be made during the next 5 years, respectively.

## *EMSL Resources*

EMSL is a national scientific user facility available to researchers worldwide from academia, industry, and national laboratories. EMSL scientific users pursue the understanding of molecular systems essential to scientific breakthroughs and discoveries for a broad set of DOE missions in energy, environment, climate, and national security. Staff at EMSL develop and maintain extensive advanced research and development capabilities that are used to generate new scientific knowledge. EMSL delivers substantial value to its scientific users by understanding their needs, creating responsive new ideas and capabilities, and delivering exceptional results—all achieved through the expertise of staff, demonstrated excellence in management and laboratory operations, and high-value partnerships with its scientific users.



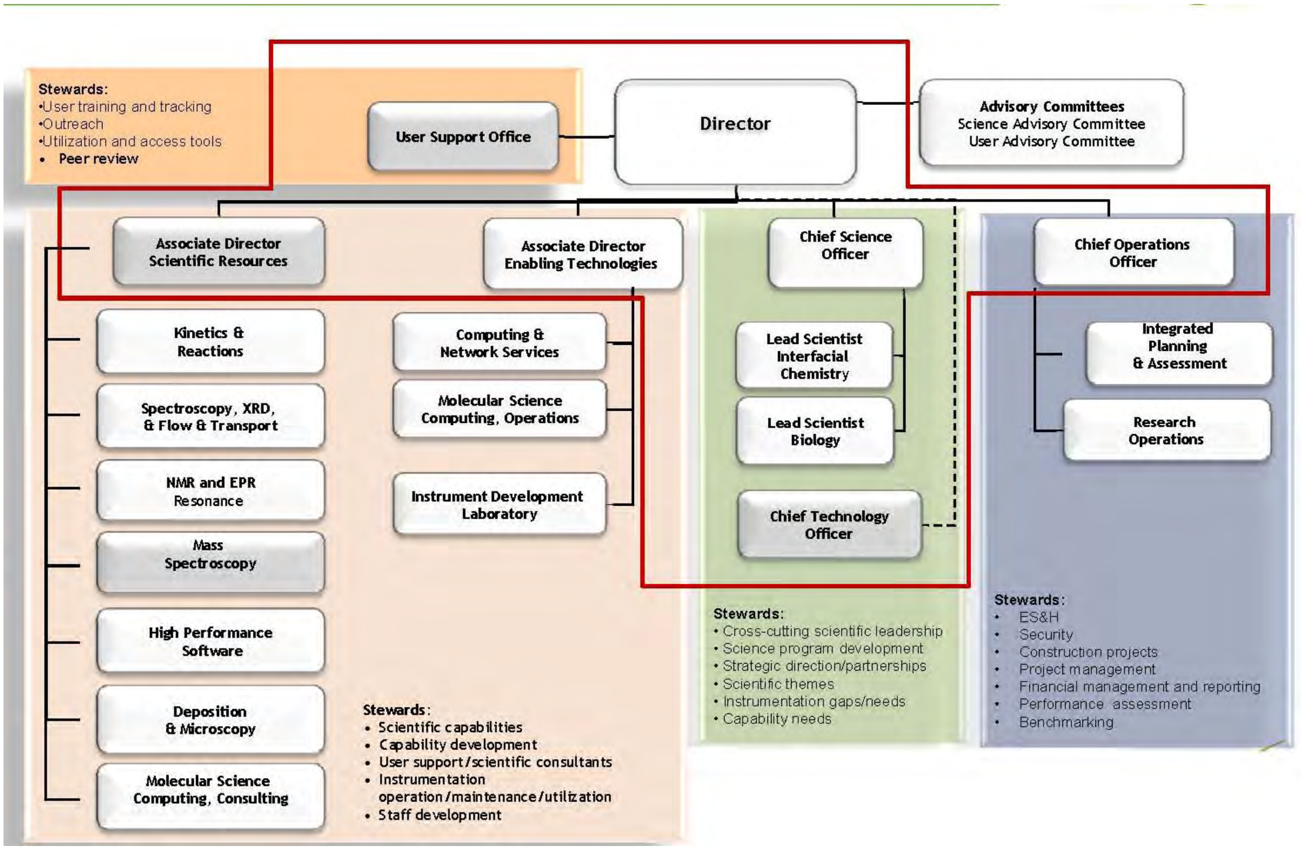
*EMSL is a DOE national scientific user facility located at Pacific Northwest National Laboratory in Richland, Washington.*

The operating budget for EMSL is provided by DOE Office of Biological and Environmental Research (BER), while the research conducted within the facility is beneficial to the DOE Office of Science and many funding agencies, including other offices within DOE, the National Institutes of Health, the National Science Foundation, and the Department of Defense.

Since beginning operations in October 1997, EMSL has provided advanced and one-of-a-kind integrated experimental and computational resources to scientists engaged in fundamental research in the physical, chemical, and biological processes that underpin environmental remediation and other important scientific issues facing DOE and the nation. In addition to physical resources, EMSL provides unprecedented technical support and expertise, providing its scientific users a highly efficient and focused resource that enhances their work.

## *Organization*

In Fiscal Year 2008, EMSL was managed by a Director, an Associate Director for Scientific Resources, a Chief Operations Officer,  a Chief Scientist and Lead Scientists, a Chief Technology Officer, and Capability Stewards (as shown in the organization chart below).



In addition, two advisory committees— the Science Advisory Committee (SAC) and the User Advisory Committee (UAC)—provide advice to the EMSL Director on longer-term scientific direction and short-term, user-related issues, respectively.

## Science Advisory Committee

The independent SAC provides objective advice on long-term science direction to the EMSL Director related to topics such as:

- EMSL's focus on national priorities and science challenges
- strategy for accomplishing EMSL's vision
- potential opportunities for transferring science to applications
- stewardship.

The SAC is comprised of distinguished scientists from academia, national laboratories, and research institutions across the United States who provide expertise in EMSL's major capability areas of biology, environmental science, molecular science, and theory. The committee reports to the Director, PNNL. Responsibilities and activities of the SAC include:

- providing advice on scientific direction for the EMSL user program
- recommending appropriate balance of instrument time for Grand Challenges, general scientific users, and capability development activities
- assisting EMSL with formulating policies related to facility scientific output, scientific impact of the EMSL user program, user access, and other issues, as needed
- performing periodic reviews of scientific impact from the various elements of the EMSL scientific user program.

The committee meets annually at EMSL and the 15 members serve staggered 4-year terms. The current members of the SAC are as follows:

- Len Spicer, Duke University (Chair)
- Mark A. Barteau, University of Delaware
- Gordon E. Brown, Jr., Stanford University
- Charles T. Campbell, University of Washington
- Marvin Cassman, Consultant
- Gregory Choppin, Florida State University
- Ian Farnan, Cambridge University
- Barbara J. Finlayson-Pitts, University of California, Irvine
- George W. Flynn, Columbia University
- David J. Galas, Battelle

- Samuel Kaplan, University of Texas-Houston Medical Center
- Julia Rice, IBM Almaden Research Center
- Peter J. Rossky, University of Texas at Austin
- James M. Tiedje, Michigan State University
- Mary F. Wheeler, University of Texas at Austin.

### User Advisory Committee

The UAC is an independent body of experts from academia, industry, and the national laboratory system that is charged with providing objective, timely advice and recommendations to EMSL leadership. The Committee reports directly to the EMSL Director and serves as the official voice of EMSL's scientific user community in its interactions with EMSL management.

The responsibilities of the User Advisory Committee include:

- providing a clear channel for the exchange of information and advice between EMSL scientific users and management
- providing a formal vehicle for EMSL scientific users to transmit concerns and recommendations to the EMSL Director
- designing and overseeing the EMSL User Meetings
- providing advice and recommendations to the EMSL Director on how to facilitate the effective use of EMSL
- nominating active scientific users for future membership to the committee.

The UAC members are:

- Theresa L. Windus, Iowa State University (Chair)
- Kerry Hipps, Washington State University (Chair Elect)
- Valérie Copié, Montana State University
- Scott Fendorf, Stanford University
- Vicki H. Grassian, University of Iowa
- Wayne Hess, Pacific Northwest National Laboratory
- Patricia M. Irving, InnovaTek, Inc.
- Anne M. Johansen, Central Washington University

- Sarah C. Larsen, University of Iowa
- Martin McIntosh, Fred Hutchinson Cancer Research Center
- Karl T. Mueller, Pennsylvania State University
- Lisa Porter, Carnegie Mellon University
- Paul G. Tratnyek, Oregon Health & Science University
- Angela K. Wilson, University of North Texas

## Science Themes

EMSL science themes are areas where EMSL can make significant scientific contributions. Current science themes build upon and expand the historical scientific expertise of EMSL. They were evaluated against key criteria including DOE and national relevance, contribution to impactful environmental molecular science, strong national science and technology programs, and the ability to grow a vibrant national user program, and they were selected with broad input and support from the scientific community and EMSL advisory committees. As scientific advances are made, the nature and elements of EMSL's science themes will evolve to reflect both scientific gains and changing societal needs. New areas will be explored and evaluated during annual business planning. EMSL's three science themes, as well as an emerging science theme, outlined in more detailed with relevant highlights given in each theme in Section 2, are (1) Atmospheric Aerosol Chemistry (emerging science theme); (2) Biological Interactions and Dynamics; (3) Geochemistry/Biogeochemistry and Subsurface Science; and (4) Science of Interfacial Phenomena.

## Proposals and Scientific User Access Modes

Users are encouraged to submit proposals in response to specific calls for proposals at defined times of the year, or in response to the Open Call at any time during the year.

### *Calls for Proposal Focus*

- **Science Theme Call for Proposals** Users are particularly encouraged to submit proposals that fit into major areas of current and growing user activity associated with scientific challenges that address topics of societal importance. To highlight these areas, Science Theme-based calls for proposals are planned to occur at least once a year. Science Theme proposals are valid for one year and may be extended twice for a total period of three years. Some EMSL resources may be principally dedicated to Science Theme proposals.

- **Computationally Intensive Research** EMSL issues a call for Computationally Intensive Research (CIR) proposals (formerly called Computational Grand Challenge Applications) once per year, provided computer time is available. The call includes research applications in biology, chemistry, climate, and subsurface science and is open to all research entities regardless of research funding source. Computer allocations for CIRs are up to three years, with the computer allocation appropriate for the scope of research to be performed.

- **Capabilities-Based Call for Proposals** The EMSL capabilities-based call for proposals generally focuses on capabilities that are not fully subscribed to following allocation to Science Theme call proposals. Proposals in response to this call are valid for one year and can be extended only once for a total open period of two years.

- **Open Call for Proposals** EMSL users may submit general-use proposals at any time. This type of proposal may not be extended and will be valid for only one year. A new proposal will be required each year. However, users may submit to the Open Call to get started and resubmit to the Science Theme call for longer access.

## *Types of Proposals*

- **General.** Use of existing EMSL resources typically falls into the general use category. General use proposals may be submitted to EMSL at any time throughout the year, and they are evaluated by peer review before research can begin. Proposals may be from individuals or groups who need access to EMSL to carry out their research, using existing equipment at EMSL. The scope of a general use proposal can vary from a single experiment proposal to full project proposal (valid for multiple visits and substantial access to a range of equipment extended over multiple years). Individual and group proposals, including collaborative proposals with EMSL staff, are encouraged.

- **Partner.** Partner proposals are submitted by individuals or groups who wish to partner with EMSL staff to enhance an existing capability or develop and build unique new capabilities that enhance EMSL's user program. Capability development efforts that support environmental molecular sciences and which utilize collaborative multidisciplinary teams, pooled or leveraged resources, unique operating environments, or other resources which may be beyond those available to individual researchers or teams are encouraged. Partner proposals are intended to leverage expertise, capability, and resources that maximize impact for EMSL, the partner, and future users. In return for co-development, EMSL partner users may have priority access to the new capability for a negotiated and specified period (subject to EMSL Advisory Committees review and approval). Proposals may be in response to a specific call or submitted at any time. The award and timing of EMSL Partner Projects are contingent upon EMSL strategic needs and the availability of EMSL resources.

  A two-page Letter of Intent (LOI) is used to initiate a dialog with EMSL's Chief Technology Officer on suitability, interest, and strategic need for the capability. A Partner user is encouraged to work with appropriate EMSL Capability Stewards or other technical contacts in preparing the Letter of Intent, which should include initial discussion of need, approach, resources, partner contributions, impact, and proposed team.
  A Letter of Intent may be submitted by a partner user at any time to emsl@pnl.gov, and will be reviewed by a panel consisting of the Chief Technology Officer, the Chief Science Officer, the Associate Director for Scientific Resources, and the Lead

Scientists. Review criteria will include strategic alignment, user/scientific impact and need, and resource and time requirements. Interaction, deliberation, and refinement of concepts with the Committee and/or EMSL staff should be expected during the LOI review process. Upon review and approval, the Chief Technology Officer or delegate will contact the partner user and request a full proposal, along with specific needs, considerations, or contacts to be addressed.
Full Partner Proposals (6-page maximum) are to be submitted to the EMSL User Portal, and will detail specific needs, considerations, or contacts to be addressed. Partner users are encouraged to work with EMSL staff in refining and developing a full proposal that meets identified EMSL capability needs and is consistent with EMSL strategy, science themes, and technology thrusts.

Full proposals will be reviewed by (selected) members of EMSL's advisory committees (Scientific Advisory Committee, User Advisory Committee) and an EMSL panel consisting of the Chief Technology Officer, the Chief Science Officer, the Associate Director for Scientific Resources, selected Lead Scientists, and other ad-hoc members as may be required for technical evaluation. Review criteria will include strategic alignment, user/scientific impact and need, and resource and time requirements. Additionally, all meritorious proposals will be reviewed by the EMSL Chief Operations Officer as part of the approval process. The Chief Technology Officer will be responsible for communicating final approval decisions to the proposal authors.

### *Resource Owner*

Proposal authors requesting to use capabilities that they co-own may select Resource Owner as the proposal type. EMSL will verify that this request is valid based on the current agreement with EMSL. Proposals that are submitted as Resource Owner are subject to internal management and safety reviews, and usage will be tracked. Proposals accepted as Resource Owner are valid for one year and can be extended twice for a total open period of three years.

### *Standard and Rapid Access*

- **Standard Access.** Standard access to EMSL facilities can vary from a single visit, single experiment proposal to a full project proposal (valid for multiple visits and substantial access to a range of equipment extended over multiple years). Prior to any performing any work, a proposal must pass peer review. This is the most common mode of access to EMSL capabilities.

- **Rapid Access.** In limited cases, users may need access to EMSL capabilities where rapid turnaround of data is required (e.g., thesis work, project progress, and paper publication or proposal preparation). If approved, a rapid access proposal will be valid for no more than one month of EMSL use. These proposals must clearly justify why rapid access is needed. Work on proposals can be started subject to instrument and resource availability and approval of the Capability Steward. Proposals will undergo internal peer review which will be conducted as work is initiated. However, all other reviews, including those by Environmental Safety & Health and the business office, must be complete before usage can begin. If users need rapid access for research that they may want to continue, they may also submit (possibly at the same time) a standard access proposal.

### *Non-Proprietary and Proprietary Research*

- **Non-Proprietary Research.** Research and equipment use at EMSL where the results and information are fully disclosed and disseminated are considered nonproprietary. Authors of nonproprietary proposals may retain rights to intellectual property (IP) resulting from the use of EMSL, but the government is granted a nonexclusive license to use the IP.

- **Proprietary Research.** EMSL facilities can be used for proprietary research. The U.S. Department of Energy (DOE) requires that such work pay full-cost recovery of the facilities used, which includes, but is not limited to, labor, equipment usage, consumables, materials, and EMSL staff travel.

### *Calls for Proposals in Fiscal Year 2008*

- EMSL's third annual Science Theme Call for Proposals closed in May 2008. EMSL received 120 proposals, 25 of which involved teams that had not previously used the facility. In addition to the science theme proposals, EMSL received 5 letters of interest for Partner Proposals and 15 letters of intent for Computationally Intensive Research Projects (formerly Computational Grand Challenges).

- Under EMSL's Open call, 72 proposals were submitted, of which 64 were accepted, including 28 Rapid Access requests. In addition, seven Computationally Intensive Research letters-of-intent were received.

## EMSL Scientific Grand Challenge

Since 2004, EMSL has been challenging the traditional approach to research with its Scientific Grand Challenges—complex, large-scale scientific and engineering problems with broad scientific and environmental or economic impacts whose solution can be advanced by applying high-performance scientific techniques and resources. EMSL Scientific Grand Challenges differ from typical research projects in that they are performed by multi-institution (universities, other federal laboratories, and industry), outcome-driven multidisciplinary teams that use a wide variety of EMSL's cutting-edge resources.

EMSL's highly successful Scientific Grand Challenge in Biogeochemistry ended in Fiscal Year 2007, while work continued on the Membrane Biology Scientific Grand Challenge, as discussed below.

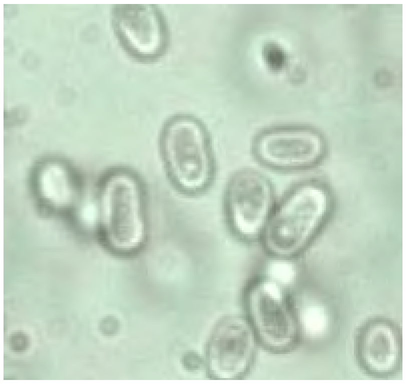
### *Membrane Biology Scientific Grand Challenge*

Dr. Himadri Pakrasi from Washington University in St. Louis is leading a Scientific Grand Challenge in membrane biology that uses a systems approach to understand the network of genes and proteins that govern the structure and function of membranes and their components responsible for photosynthesis and nitrogen fixation in cyanobacteria (blue-green algae). A systems approach integrates all temporal information into a predictive, dynamic model to understand the function of a cell and the cellular membranes. These microorganisms make significant contributions to harvesting solar energy, planetary carbon sequestration, metal acquisition, and hydrogen production in marine and freshwater ecosystems. Cyanobacteria are also model microorganisms for studying the fixation of carbon dioxide through photosynthesis at the biomolecular level. The results of this Scientific Grand Challenge are providing the first comprehensive systems-level understanding of how environmental conditions influence key carbon fixation processes at the gene-protein-organism level. This topic was selected because it addresses critical DOE science needs, provides model microorganisms to apply high-throughput biology and computational modeling, and because it takes advantage of EMSL's experimental and computational capabilities. The following highlights illustrate the activities under this Scientific Grand Challenge in Fiscal Year 2008:

**More Proteins Visible with New Genome Annotation Approach.** A new proteomic analysis technique, developed by researchers on the EMSL's Membrane Biology Scientific Grand Challenge, has substantially contributed to annotation of gene sequences. Researchers from Washington University in St. Louis, St. Louis University, Purdue University, and Pacific Northwest National Laboratory developed an approach that synergistically sequenced the DNA of cyanobacteria *Cyanothece* 51142 and determined the proteins that the microbe produced at different times of its life cycle. The proteomics research was done at EMSL using state-of-the-art instrumentation, and the resulting data was compared to determine which of the DNA sequences produced the proteins.

In this way, the team determined where genes resided on the genome of the cyanobacteria and found a previously missed linear chromosome, common in more complex organisms. The blue-green algae, which conducts photosynthesis during the day and nitrogen fixation at night, could make significant contributions in producing ethanol and hydrogen, reducing the need for fossil fuels. "This is the first time anything like this has been found in photosynthetic bacteria. It's extremely rare for bacteria to have a linear chromosome," said team leader Himadri Pakrasi, who leads the EMSL Grand Challenge.

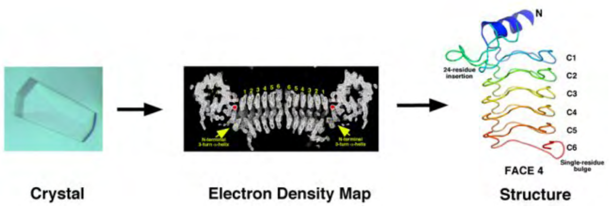
This new approach can provide insights into microbial genes and proteins, microbial functions, and microbial communities, which could hold the key to reactions of interest in the energy, environmental, and health arenas. This work is part of EMSL's crosscutting work to predict biological functions from molecular and chemical data. In addition, understanding microbial functions, such as in cyanobacteria, can be valuable in producing hydrogen and ethanol, turning these microbes into fuel factories.



*Simultaneous proteomic and genomic technique leads to discovery of rare, linear chromosome in cyanobacteria.*

**Citation:** Welsh EA, M Liberton, J Stockel, T Loh, T Elvitigala, C Wang, A Wollam, RS Fulton, SW Clifton, JM Jacobs, R Aurora, BK Ghosh, LA Sherman, RD Smith, RK Wilson, and HB Pakrasi. 2008. "The Genome of *Cyanothece* 51142, A Unicellular Diazotrophic Cyanobacterium That Is Important In The Marine Nitrogen Cycle." *Proceedings of the National Academy Sciences Early Edition*, September 15.

**New Study Reveals Protein "Towers."** Using EMSL, scientists determined the crystal structure of a protein from the blue-green bacteria, *Cyanothece*. The protein, Rfr23, belongs to a large family of proteins called pentapeptide repeat proteins (PRPs), so named for the presence of tandem repeats of five similar amino acids. Four tandem repeats form a "square" coil and in turn the coils stack together to form four-faced protein "towers."

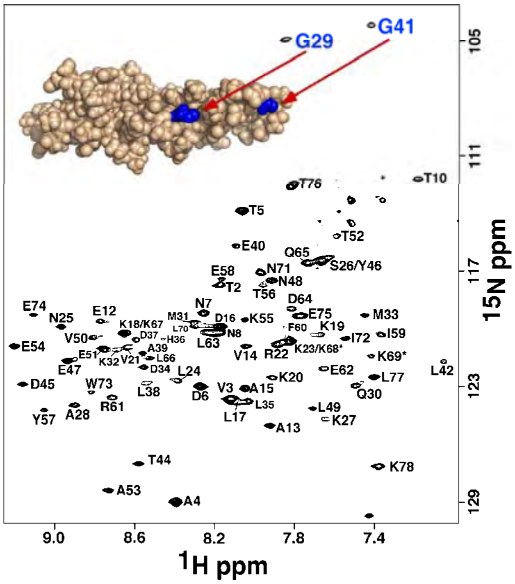


*Summary of the steps to determine the crystal structure for Rfr23. The first step is to grow a crystal, shown here highly magnified for Rfr23. X-ray diffraction data is then collected on this crystal at a synchrotron and the diffraction data converted into an electron density map. The structure of Rfrr23 is then "built" into the electron density map. Here, the structure is presented as a cartoon colored spectrally (red to violet) from the C-terminus. The structure is dominated by an Rfr-fold, composed of nearly six complete coils, C1-C6, that is capped at the N-terminus with a small a-helix.*

The biological purpose of PRPs is not yet known. However, these proteins are prolific in blue-green bacteria such as *Cyanothece* – an organism that uses circadian rhythms to perform photosynthesis during the day and nitrogren fixation at night. Consequently, many scientists hypothesize that PRPs may play a role in the bacteria's circadian lifestyle. *Cyanothece* is of interest because it naturally absorbs carbon dioxide and sequesters it as organic carbon. Furthermore, a by-product of its nocturnal nitrogen fixation is hydrogen gas, a potential fuel. Regardless of their purpose, insights into PRP's structure may provide ideas for designer or tailored proteins.

Scientists from Washington University-St. Louis, Brookhaven National Laboratory, and Pacific Northwest National Laboratory determined the crystal structure of Rfr23 at 2.1 Å resolution. The crystals were grown at PNNL, and data was collected at the National Synchrotron Light Source at BNL. Biophysical studies of the PRPs in solution were done with EMSL nuclear magnetic resonance spectrometers. In studying the structure, the scientists discovered that the orientation of the protein's side chains were related to their position in the pentapeptide repeat. The biophysical properties of a protein are determined by these side chains, and hence, by selective positioning the side chains on the tower, researchers could design new proteins with specific physical or chemical properties.
The team will now study other PRPs in *Cyanothece* to obtain clues towards the protein's raision d'etre.

**Citation:** Buchko GW, H Robinson, HB Pakrasi, and MA Kennedy. 2008. "Insights into the structural variation between pentapeptide repeat proteins—Crystal structure of Rfr23 from *Cyanothece* 51142." *Journal of Structural Biology* 162(1):184-192.



*The assigned $_{1}$H-$_{15}$N HSQC spectrum for cce_0567 with the crystal structure of the protein (3CSX) is shown near the top. Understanding the function of this protein may help scientists use blue-green algae for producing energy and sequesteringcarbon.*

**Scientists solve structure of a mysterious protein found in cyanobacteria.** Scientists from the Pacific Northwest National Laboratory and Brookhaven National Laboratory have determined the crystal structure for the 78-residue protein cce_0567 from the cyanobacteria *Cyanothece sp. PCC 51142*. Studies suggest that the protein may play a role in nitrogen fixation and/or the circadian control of nitrogen fixation. Nitrogen fixation is the rate-limiting step in the growth of cyanobacteria. Understanding the proteins involved in nitrogen fixation could help unlock the mysteries of how to efficiently turn this ubiquitous algae into a carbon-neutral fuel. Using state-of-the-art resources at EMSL, the nuclear magnetic resonance chemical shift assignments for cce_0567 were made using EMSL's 500-, 600-, 750-, and 800-MHz NMR spectrometers. The $^{1}$H -$^{15}$N HSQC spectrum is a "fingerprint" for the protein's conformation. The assignment of the $^{1}$H -$^{15}$N HSQC spectrum is an important step in probing the biological function of cce_0567. Perturbations to these chemical shifts occur when other molecules are added to the solution. The perturbations are indicative of substrate binding. Following such chemical shifts allows researchers to identify protein-substrate interactions and then map them on to specific locations on the protein's surface using the structure determined by crystallographic methods.

Understanding the structure of cce_0567 and other cyanobacteria proteins paves the way for further scientific inquiry, including biochemical experiments, into ubiquitous blue-green algae. It also is part of a broader endeavor to harness bacteria to efficiently produce hydrogen, a potential clean-burning alternative fuel.

**Citation:** Buchko GW, and HJ Sofia. 2008. "Backbone $^{1}$H, $^{13}$C, and $^{15}$N NMR Assignments for the *Cyanothece 51142* Protein cce_0567: A Protein Associated with Nitrogen Fixation in the DUF683 Family." *Biomolecular NMR Assignments* 2(1):25-28.

# EMSL Highlights

## Major EMSL Activities

**MPP2 Removed; Chinook Installed.** In July 2008, EMSL staff made room for one of EMSL's newest and heavily anticipated additions—Chinook, a $24-million HP-developed supercomputer that will support chemistry, biology and environmental computation and is expected to have a total peak performance of about 163 teraflops.

*Before installing Phase 2 of Chinook, EMSL staff removed about 25 miles of communications cables that once passed data between the older supercomputer's nodes.*

HP began delivery of Chinook to EMSL in March, first populating a newer addition of the computing center that was completed in January 2007. With additional pieces of the system delivered in July, it was time to remove the older system, which was recycled. As of August 1, the components delivered and installed in March fully absorbed the old system's workload, and the new system began running nearly all science codes the older system had previously run.

The system is targeted to be accepted in early Calendar Year 2009.

*The family of Mike White stands next to the plaque erected in his honor at EMSL. From left: daughter RaeAnne, wife Gwen, son Mark, daughter-in-law Melissa, and son Paul.*

**New Office Pod Dedicated to Memory of Distinguished User.** On April 28, 2008, 25,000 square feet of new office space at EMSL was dedicated to the memory of Professor J. Mike White, a Robert A. Welch Chair of Materials Chemistry at the University of Texas at Austin, founding Director of the Pacific Northwest National Laboratory's Institute for Interfacial

Catalysis, and distinguished EMSL user.

White passed away unexpectedly on August 31, 2007, while visiting his son in Oklahoma City, Oklahoma. During his lengthy career, he pioneered research in many areas of surface chemistry, catalysis, the dynamics of surface reactions, and photoassisted surface reactions.

White's wife Gwen; children Mark, Paul, and RaeAnne; daughter-in-law Melissa; and longtime research associate Yangming Sun attended the dedication, along with more than 100 of White's colleagues, including former EMSL Director Bill Rogers and Charlie Campbell, professor of chemistry at the University of Washington and member of EMSL's Science Advisory Committee. Both had been mentored by White early in their careers. A plaque memorializing White was unveiled during dedication of the $4.8-million wing, which was completed in December 2007. The space houses more than 90 staff and users who began moving into the wing in February 2008.

**EMSL Hires Teller as Associate Director.** On August 18, 2008, Dr. Raymond Teller joined EMSL as the Associate Director for Scientific Resources. In his new position, Ray is responsible for oversight of EMSL's scientific capabilities and staff. He is helping to establish and guide strategies for revitalizing EMSL's capabilities, achieving EMSL's scientific vision, and bolstering user outreach.

*Ray Teller*

Ray previously served as Director of the Intense Pulsed Neutron Source, a DOE Office of Basic Energy Sciences-funded national user facility at Argonne National Laboratory. At IPNS, he provided oversight of 90 staff and a $17 million budget, and he established many partnerships and collaborations within the academic community, funding agencies, industrial partners, and other international and U.S. national laboratories.

Ray replaces former Associate Director Gordon Anderson, who joined the Biological Separations and Mass Spectrometry within PNNL's Fundamental and Computational Sciences Directorate in August 2007.

## *EMSL Staff and Scientific User Highlights*

In 2008, EMSL staff and scientific users received continued recognition for progress in development of state-of-the-art capabilities and expertise, and for their professional contributions.

*From left to right: Allison Campbell, EMSL Director; Dave Koppenaal, EMSL Chief Technology Officer; and university Chancellor Mark Wrighton. (Photo courtesy of Mary Butkus/Washington University in St. Louis)*

**Pakrasi honored with Freiberg Award.** Himadri Pakrasi, lead investigator of EMSL's Membrane Biology Grand Challenge was installed in early October as a George William and Irene Koechig Freiberg Professor of Biology in Arts and Sciences at Washington University in St. Louis. The professor of biology and energy at the university received the award that was established in 1983 to honor faculty in the field of biology who have demonstrated leadership in research and teaching. Pakrasi's research involves systems biology, photosynthesis, membrane biology, metal homeostasis, redox processes, and genomics. In 2005, he forged a partnership between the university and EMSL to form one of EMSL's first Scientific Grand Challenges, addressing membrane biology. This Grand Challenge, which involves researchers from six institutions, has led to determination of a new class of proteins that transport carbon and nitrogen across cyanobacteria membranes, providing insight into nature's methods for carbon sequestration and nitrogen fixation.

*Julia Laskin*

**Laskin receives Presidential honor.** EMSL user Julia Laskin (Pacific Northwest National Laboratory) received the U.S. government's highest honor for researchers at the beginning of their careers when she accepted the Presidential Early Career Award for Scientists and Engineers at the White House on November 1, 2008. A senior research scientist, Laskin was honored for her work in fundamental reaction kinetics and ion surface reactions.

**Laskin honored with Biemann Medal.** Laskin also received the Biemann Medal, the highest honor granted to a young scientist by the American Society for Mass Spectrometry. Laskin accepted the award at the ASMS annual conference June 3, 2008, in Denver, Colorado, where she also delivered a lecture on her research to the nearly 7,000 scientists attending the conference. The international award recognizes Laskin's contributions to better understanding the activation, fragmentation, and deposition of large molecules when they collide with surfaces. Her research is of interest to the scientific community and directly advances DOE goals to develop biomaterials and biological processes for clean energy production, as well as to create biologically inspired systems, novel catalysts, and biosensors. Other findings by Laskin and her collaborators provide fundamental insights into the analysis of complex molecules present in biofuels, petroleum, and aerosols.

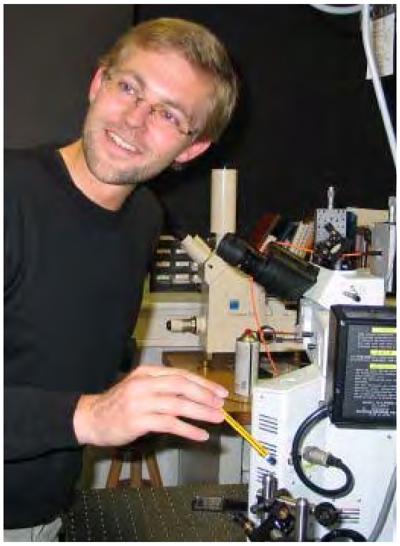
*Greg Exarhos*

**Exarhos elected President of AVS.** Greg Exarhos, an EMSL user from Pacific Northwest National Laboratory, was elected President of the AVS: Science and Technology of Materials, Interfaces, and Processing. Founded in 1953, this not-for-profit society was focused on vacuum science and technology, critical in the early development of vacuum tubes, enabling radio broadcasting, radar, and other technologies. Today, the society has broadened its scope to include such technologically relevant areas as surface science, electronic and magnetic materials, nanoscience, and biomaterials.Exharhos' work has been recognized internationally and has opened new venues in optical and electronic coatings, new materials designed at the nanoscale, multifunctional ceramics, and hybrid polymer composites. In addition, Exarhos is actively involved in the operations side of the society. An AVS Fellow, he has been elected to the Board of Directors, served as Chair of the Long Range Planning Committee, and has served as Chair of numerous society-sponsored meetings. He currently serves as the Publications Chair and oversees several journals, including the new open access journal, *Biointerphases*, which he launched for the society in 2006. Exarhos' election was announced at the AVS International Symposium in Seattle in October 2007. He began his three-year term in January 2008.

Desmond Smith

Dick Smith

**Pair of Smiths named to Scientific American 50 list.** EMSL users Desmond Smith (University of California in Los Angeles) and Dick Smith (Pacific Northwest National Laboratory) shared the honor of being named to the 2007 Scientific American 50 list in January 2008. Assembled by *Scientific American*'s Board of Editors, the list honors 50 outstanding people or teams for their achievements and leadership in shaping established and emerging technologies. Both were honored for their work developing new methods for rapid mapping of gene and protein expression patterns in the mammalian brain. Using resources at EMSL and other laboratories, these two scientists and their collaborators are developing analytical methods and technologies, including voxelation and gene expression tomography, to detect patterns in the transcriptome and proteome—the complete set of RNA that creates the chemical "blueprint" for producing proteins and the complete set of proteins produced—in the brain. Using high-throughput mass spectrometers and other instruments available at EMSL, they are decoding the conceptual wiring diagram of the genome, which gives rise to proteins that are responsible for the neuronal wiring diagram of the brain. Eventually, this research may help to identify patterns that indicate the early stages of brain impairment, such as Alzheimer's, Parkinson's, and other neurological diseases. Many biomedical researchers believe that detecting disease states before symptoms occur is key to reversing many as-yet-incurable diseases.

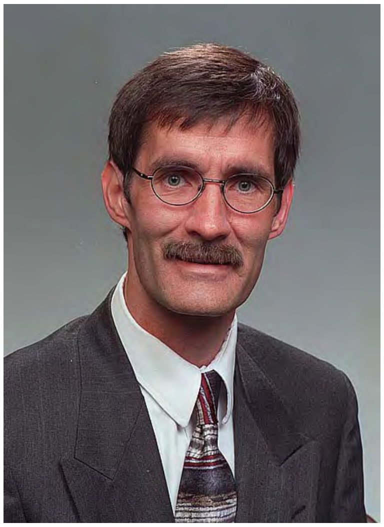


Markus Raschke

**Raschke receives prestigious NSF Career Award.** EMSL user Markus Raschke, an Assistant Professor in the Department of Chemistry at the University of Washington, has received a prestigious Career Award from the National Science Foundation. The Career Award is one of the NSF's most prestigious awards in support of the early career development activities of those teacher-scholars who most effectively integrate research and education within the context of the mission of their organization. Raschke received the award from the NSF's Division of Chemistry for the research project "Spatio-Temporal Imaging and Spectroscopy of Ultrafast Electron and Vibration Dynamics on the Nanoscale." As part of this award, he will receive $640K over the next 5 years to further his research. Raschke is using EMSL's new Focused Ion Beam/Scanning Electron Microscope as well as clean room microfabrication capabilities to support NSF-funded research addressing fundamental questions about the electron and vibration dynamics of nanoconfined systems. To achieve simultaneous ultrahigh temporal and nanometer spatial resolution, he and his group are combining femtosecond time-resolved spectroscopy with optical near-field microscopy techniques. The local optical field enhancement of scanning probe tips is providing the necessary spatial field confinement. The proposed work under this award includes probing the electron dynamics in individual plasmonic nanocrystals to provide insight into the time scale and efficiency of different relaxation channels and their correlation with structural parameters. Similarly, studying the vibrational dynamics is allowing the researchers to distinguish spatial and temporal decoherence in molecular nanostructures.

**Zhang invited to NAE, NAS symposia.** EMSL researcher Yanwen Zhang was invited by the National Academy of Engineering to attend the 2008 German-American Frontiers of Engineering Symposium. The symposium, to be held April 25 – 27, 2008, at the National Academies' Beckman Center in Irvine, California, is organized by the NAE and the Alexander von Humboldt Foundation. The symposium hosted about 60 outstanding engineers, generally not older than 45, from U.S. and German industry, universities, and government labs to discuss leading-edge research and technical work across a range of engineering fields. Zhang was also invited by the National Academy of Science to attend the 2008 German-American Kavli Frontiers of Science Symposium, held June 11-14, 2008, in Potsdam, Germany. The NAS symposia are attended by approximately 70 scholars under 45 years of age, by up to a dozen senior colleagues, and by several science writers. Participation at the symposium is split evenly between the Germans and Americans, and the symposium alternates every year between Germany and the United States. Participants include leading researchers from academic, industrial, and federal laboratories all fields.

*Yanwen Zhang*



*Mark Engelhard*

**Engelhard appointed as AVS Publications Chair.** EMSL researcher Mark Engelhard was appointed Publications Committee Chair for AVS: Science and Technology of Materials, Interfaces, and Processing. Founded in 1953, this international society was focused on vacuum science and technology, critical to developing vacuum tubes, enabling radio broadcasting, radar, and other technologies. Today, the society has broadened its scope to surface science, electronic and magnetic materials, nanoscience, biomaterials and other relevant areas. Communications is an important part of the mission of the society, which publishes 4,000 to 5,000 pages of scientific information in the AVS Monograph Series and four journals: *Journal of Vacuum Science & Technology A,* a top 10 journal in the materials sciences and coatings field; *Journal of Vacuum Science & Technology B; Surface Science Spectra;* and the relatively new journal, *Biointerphases* During his 2-year term leading the Publications Committee, Engelhard will serve as the chair of the editorial boards for these journals and will also recommend candidates for leadership positions on the journals. He will work with the staff of each journal to maintain the high volume of top-notch articles. Further, he will oversee the publications budgets, ensuring costs are kept within the limits of this not-for-profit society. Engelhard's appointment by John N. Russell, Jr., president of society, was announced at the AVS International Symposium in Seattle in October 2007 with his term beginning in January 2008.


*Gerard Parkin*

**Parkin receives ACS award.** EMSL user Gerard F. R. Parkin, chemistry professor at Columbia University, received the 2008 American Chemical Society Award in Organometallic Chemistry. This award, established in 1983, recognizes recent achievements in the study of compounds that contain bonds between carbon and a metal; compounds that are important in both industrial catalysts and human enzymes. Parkin is known for his work on the development of models for the active sites of zinc enzymes. Because of the critical role zinc plays in biology – zinc is the second most abundant trace element in humans after iron, Parkin's models provide a deeper understanding of the structures and mechanisms of these important proteins. As part of his efforts, he collaborated with the Ellis group at Pacific Northwest National Laboratory, utilizing EMSL's unique low-temperature solid-state nuclear magnetic resonance spectroscopy methods, as well as the supercomputer for advanced modeling and simulations. This collaborative effort utilizing metalloproteins is just one example of Parkin's outstanding research program. Beyond his scientific studies, Parkin was recognized for his intense passion for chemistry. His creativity, rigor, and insight can be seen in his laboratory as well as in his many publications. Further, his ability to communicate the often complex nature of organometallic chemistry to his students and peers with ease and humor was noted.


*Bruce Kay*

**Kay appointed to BESAC.** EMSL user Bruce D. Kay, Pacific Northwest National Laboratory, was recently appointed to the Basic Energy Sciences Advisory Committee. This committee helps solve challenging scientific and technical issues for BES, part of the U.S. Department of Energy's Office of Science. Through BES, researchers expand the scientific foundations for energy technologies and understand and mitigate the environmental impacts of energy use. As a part of the 25-member committee, composed of experts from academia, national laboratories, and other institutions, Kay will make recommendations on research and facilities priorities, appropriate balance among scientific disciplines, and collaboration among research institutes and industries. Undersecretary for DOE's Office of Science Dr. Raymond Orbach selected Kay for this assignment. He was chosen for his internationally recognized leadership in the chemical sciences. At EMSL, he conducts BES-funded research in condensed phase chemical kinetics and molecular dynamics aimed at gaining a detailed physical understanding of the molecular-level interactions responsible for phase transitions and catalytic chemical reactions.

Don Baer

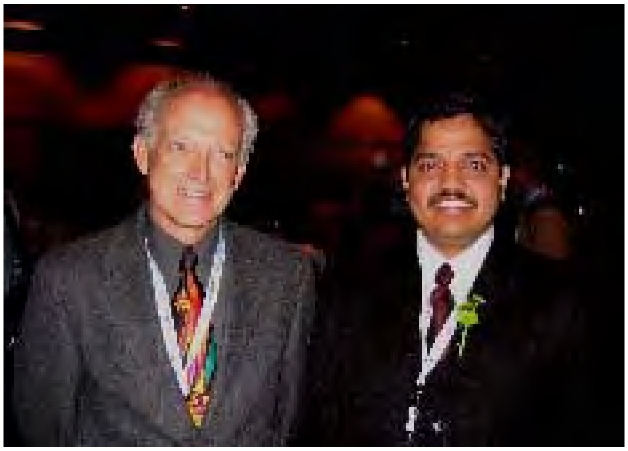
**Baer elected to third ASTM term.** Don Baer, EMSL's Lead Scientist for Interfacial Chemistry, was elected to a third term as Chair of the ASTM International Committee E42 on Surface Analysis. The committee has jurisdiction over some 25 standards for surface analysis methods and is one of 136 ASTM technical standards writing committees. He began serving the 2-year term—his final—on January 1. Baer is internationally known for the application of surface analysis methods to examine corrosion processes and the reactive properties of oxide and mineral surfaces. Since joining the Pacific Northwest National Laboratory—on whose campus EMSL resides—he has specialized in the use of surface-sensitive techniques to study how the interactions of a material with its environment alter material properties. Much of his research has involved understanding the roles of surface impurities or contaminants in chemical reactivity, and his current work involves understanding the reaction properties and environmental variability of nanoparticles.

**Thevuthasan appointed as AVS committee chair.** EMSL researcher Theva Thevuthasan was appointed Chair of the Short Course Executive Committee for AVS: Science and Technology of Materials, Interfaces, and Processing. Through this committee, the international society provides scientists, engineers, and technicians with classes in vacuum and equipment technology, materials and interface characterization, and materials processing. A frequent volunteer and long-time mentor, Thevuthasan served on the Short Course Executive Committee for about 10 years in different capacities. As the committee chair, Thevuthasan ensures the quality of more than 60 courses, such as "Comprehensive Course on Surface Analysis" and "Fundamentals of Vacuum Technology." During his 3-year appointment, Thevuthasan is eager to continue the society's work to increase short course participation, which began to decline in 2001 based on changes in the semiconductor business. He is leading the committee in developing four focused educational programs this year, based on input from potential and past students.

Theva Thevuthasan

Paul Tratnyek

**Tratnyek receives OHSU Faculty Senate Award.** EMSL User Advisory Committee member Paul Tratnyek received a 2007 Oregon Health and Science University Faculty Senate Award. This award recognizes OHSU faculty members who have demonstrated a sustained and significant record of meritorious academic accomplishments. Tratnyek, a professor in the department of environmental and biomolecular systems at OHSU's OGI School of Science and Engineering, was recognized for exceptional efforts in support of the university's mission in collaboration. He was cited for his skill at finding ways to bring things together—whether carbon atoms, disparate disciplines, or people—and contributing to the collaborative environment at OHSU. His research activities have been focused on the application of nanotechnology to basic and biomedical science in partnership with scientists at OHSU as well as other universities and the Pacific Northwest National Laboratory. He has investigated, among other things, the use of nanosized particles of iron for cleaning up contaminants in groundwater, soil and sediments. Recognizing that most new frontiers of science are at the interface between disciplines, he has been a champion of developing interdisciplinary education for students. Tratnyek received $3,500 from the OHSU Foundation as part of this award.



*Satya Kuchibhatla (right) with EMSL Lead Scientist for Interfacial Chemistry, Don Baer.*

**Kuchibhatla receives AVS Graduate Award.** Satyanarayana Kuchibhatla, a graduate student from Professor Sudipta Seal's group at University of Central Florida who is conducting research at EMSL, received an AVS Graduate Research Award for 2007. Satya is working with EMSL interfacial and nanoscale science researchers Theva Thevuthasan and Don Baer. The trio attended the AVS 54th International Symposium in Seattle, where Satya was honored during an awards assembly on October 17 and gave a presentation about his research.

Fung Suong Ou

**Former SRI student receives Foresight Award.** Fung Suong Ou, a graduate student who investigated a new method of building nanowires at Rice University, received a prestigious nanotechnology award from the Foresight Nanotech Institute in October at the Productive Nanosystems Conference in Arlington, Virginia. Ou received the Foresight Institute Distinguished Student Prize, an annual award given for the college undergraduate or graduate student whose work in nanotechnology is deemed most notable. He received the award for his work on hybrid nanowires that he pioneered.

"The research experience I had at EMSL helped me a lot and is certainly one of the main factors that made such an award possible," said Ou.

Ou conducted nanotechnology research while attending Pacific Northwest National Laboratory's Summer Research Institute for Interfacial and Condensed Phase Chemical Physics. At the Institute, he was mentored by EMSL researcher Lax Saraf and Don Baer, EMSL Lead Scientist for Interfacial Catalysis.

**Wang appointed to editorial advisory board.** Lai-Sheng Wang, a long-time EMSL user, was appointed to the 2008 Editorial Advisory Board of *The Journal of Physical Chemistry*. A professor at Washington State University Tri-Cities and an Affiliate Senior Chief Scientist at Pacific Northwest National Laboratory, Wang was selected for the three-year term on board based on his distinguished and innovative contributions to the field of atomic clusters and for pioneering work on gaseous multiply-charged anions. In this role, Wang will influence the current policies and future direction of this publication. Produced weekly by the American Chemical Society, the journal is actually three highly respected journals focused on different aspects of experimental and theoretical research of interest to physical chemists and chemical physicists.

Lai-Sheng Wang

**Dupuis elected Fellow of APS.** EMSL user Michel Dupuis (Pacific Northwest National Laboratory) was elected Fellow in the American Physical Society. The APS is a leading voice for physics, including chemical physics, in both the U.S. and international scientific communities. Founded in 1899, the society publishes several prestigious journals, including *Physical Review* and *Physical Review Letters*. Dupuis received this honor for his outstanding contributions to the development of electronic structure methods and computer codes for the simulation of molecular properties and reactivity. A Laboratory Fellow at PNNL, Dupuis has more than three decades of experience in developing computational chemistry methods and algorithms on supercomputers and applying these methods to chemical problems. Dupuis is part of several EMSL Computational Intensive Projects that are running calculations on the EMSL supercomputer, and computer codes that Dupuis developed can still be found in the EMSL flagship software NWChem.

*Michel Dupuis*

*Bill Weber*

**Weber selected as inaugural MRS Fellow.** EMSL user Bill Weber, Pacific Northwest National Laboratory, was selected as an inaugural Fellow in the Materials Research Society. This is the first year, since being founded in 1973, that the society has honored notable members for their contributions to advancing materials research. Weber received this honor for his “seminal contributions, leadership, mentoring and innovative research on defects, defect properties, ion-solid interactions, radiation effects and models of radiation damage processes in glasses and ceramics.” His research is focused on the fundamental understanding and accurate modeling of the effects of atomic-level defects and radiation on ceramics. This research is essential for advancing electronic devices, developing radiation-tolerant materials for new nuclear power reactors, and addressing concerns regarding the stability of nuclear waste.

Dick Smith

**Smith selected as AVS Fellow.** EMSL user Dick Smith—physics professor at Montana State University—was selected as a Fellow in the AVS: Science and Technology of Materials, Interfaces, and Processing. This not-for-profit society focuses on surface science, electronic and magnetic materials, nanoscience, and biomaterials. Smith received this honor for his outstanding expertise researching metal-metal interfaces. An award-winning researcher, Smith has more than 30 years of experience in investigating the structure and composition of metal-metal interfaces and studying the growth process as one metal is deposited on another. His work has been aided by the use of ion beam techniques, such as Rutherford backscattering and channeling instrumentation at EMSL. Smith credits EMSL's integration of instrumentation and expertise in aiding his research. "EMSL has both state-of-the-art facilities and a group of clever scientists who know how to use the equipment to get reliable data, and they are able to help users learn how to perform correct analysis of the results," said Smith.

Yuehe Lin

**Lin named PNNL Fellow.** EMSL user Yuehe Lin, Pacific Northwest National Laboratory, was named Laboratory Fellow, the highest rank that PNNL science and engineering staff can attain. Laboratory Fellows are chosen for establishing careers of sustained, highest-quality research and development in science or engineering fields. They are recommended by the Laboratory Fellow Review Committee, which has representation from across PNNL. Lin is a longtime contributor to the fields of chemical sensors and biosensors and biomedical nanotechnology. He and his co-workers have established a research program at PNNL for the development of nanomaterial-based chemical sensors and biosensors for environmental, homeland security, and biomedical applications. They have also developed functional nanomaterials for fuel cells, drug delivery, and environmental remediation applications.

Keqi Tang

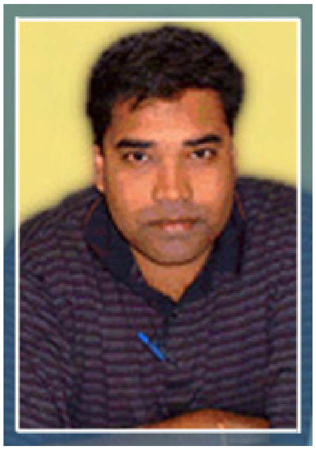
**Tang named PNNL Inventor of the Year.** EMSL user Keqi Tang was named Pacific Northwest National Laboratory Inventor of the Year for 2007. The PNNL Inventor of the year award recognizes innovation that has resulted in the creation of intellectual property or the potential to create intellectual property. Tang was chosen for his work in developing novel innovations in the field of mass spectrometry. He currently has 19 currently pending or issued patents and has been named inventor on 11 patent applications since 2006. Tang is known as a hands-on inventor who diligently ensures that conceptual ideas are implemented in working instruments. He has focused on the design, fabrication and testing of new ion sources, ion optics systems, and gas phase separation methods to improve sensitivity and resolution in mass spectrometry. His intellectual property has garnered 8 licenses with commercial firms.

**Wiley invited to write column for** Steven Wiley, EMSL's Lead Scientist for Biology, accepted an invitation from *The Scientist* to write a monthly column on his thoughts and opinions about life sciences. His first column appeared in the January 2008 issue. Wiley was asked to write the column because of the fresh perspectives he brings as well as his scientific credibility. In particular, the journal's editorial board was impressed with his collaborative research into large-scale protein-protein interactions and cell signaling networks at EMSL as well as his work as the Director of Pacific Northwest National Laboratory's Biomolecular Systems Initiative. While his credentials helped make him a logical choice for this task, it was his lively writing style that had the journal's editors repeatedly ask him to take over the column. "They thought I was entertaining," he noted.

Steve Wiley

**Wiley appointed to Burroughs Wellcome Fund Committee.** Wiley was also appointed to an advisory committee for the Burroughs Wellcome Fund, which is a private, philanthropic organization. The committee will evaluate applications for their Institutional Program Unifying Population and Laboratory-Based Sciences. This program was created to bridge the gap between population approaches to human health and basic biomedical research. The program provides grants of $500,000 per year for 5 years to stimulate graduate student training programs and to bring together scientists working in fundamental sciences as well as those in schools of medicine and public health. As a member of the advisory committee, Wiley will evaluate and provide guidance on the directions and progress of the institutional program. This includes reviewing numerous grant proposals and attending conferences, such as an upcoming workshop on microbial systems in Denver, Colorado.

**Seal elected to ASM Class of Fellows.** EMSL user **Sudipta Seal,** University of Central Florida, was elected to the 2008 Class of Fellows by the ASM International Board of Trustees. The honor of Fellow represents recognition of Seal's distinguished contributions in the field of materials science and engineering, and helps to develop a broadly based forum for technical and professional leaders to serve as advisors to the Society. He was honored at the Convocation of Fellows held during the ASM Awards Dinner on Tuesday, October 7, 2008, in Pittsburgh, Pennsylvania.



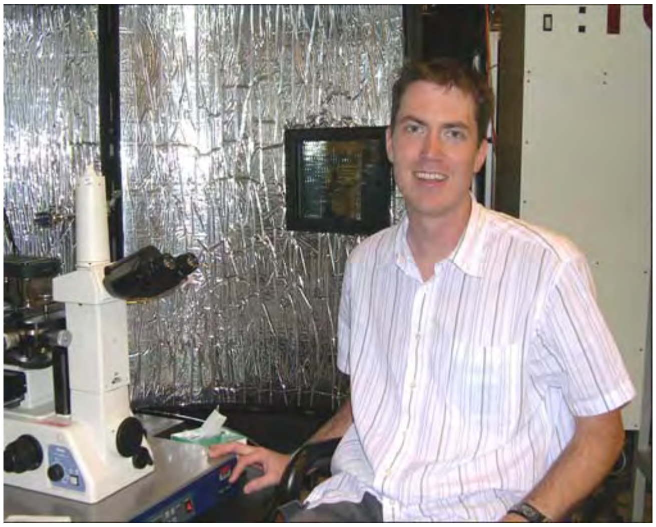
*Sudipta Seal*

*Ljiljana Paša Tolić*

**Paša Tolić co-author of lauded paper.** EMSL researcher **Ljiljana Paša Tolić** was among the authors of a paper that was selected to receive *International Immunology's* Outstanding Merit Award for the article of exceptional value for 2007. The paper is "Preferential Recognition of a Microbial Metabolite by Human V2V2 T Cells INTIMM-06-0286.R1" [19(5):657-673, published May 2007], authored by Kia-Joo Puan, Chenggang Jin, Hong Wang, Ghanashyam Sarikonda, Amy M. Raker, Hoi K. Lee, Megan I. Samuelson, Elisabeth Märker-Hermann, Ljiljana Paša Tolić, Edward Nieves, José-Luis Giner, Tomohisa Kuzuyama, and Craig T. Morita, the latter an EMSL user from the University of Iowa. The editors of the journal present this award in special recognition of the article deemed to exhibit the highest distinction in immunological research.

*Zhenrong Zhang*

**Zhang receives M.T. Thomas Award.** EMSL user Zhenrong Zhang, Pacific Northwest National Laboratory, was selected as the 2007 recipient of M.T. Thomas Award for Outstanding Postdoctoral Achievement. The award recognizes her scientific contributions that promote the mission of EMSL. Her new experimental method and resulting measurements are important steps in material science and may lead, among other things, to designing and controlling catalysts that produce clean-burning hydrogen fuel. Zhang was selected for the award for achieving the first atomically resolved high-temperature scanning tunneling microscopy measurements and resulting insights on the understanding of the adsorbate reactivity and diffusion dynamics on $TiO_2$. This oxide is an extremely promising material with applications in such diverse and technologically important areas as catalysis, air purification, and wastewater treatment. She was honored at a reception on August 6, 2008, and gave a presentation on her research on September 16, 2008.



*Zachery Oestreicher in front of EMSL's atomic force microscope.*

**Oestreicher receives NSF grant.** EMSL user Zachery Oestreicher, graduate student at The Ohio State University, was awarded a National Science Foundation grant to study protein-mineral/bacterial-mineral interactions in Japan this summer. The NSF East Asia and Pacific Summer Institutes for U.S. Graduate Students and the Japan Society for the Promotion of Science provided the grant to help students learn more about science and engineering in other countries and initiate scientific relationships that will better enable future international collaboration. For eight weeks, Oestreicher will work at the Kanazawa University with Professor Yoshihiro Fukumori studying proteins associated with the *Magnetosprillum magnetotacticum* magnetosome. The magnetosome is an organelle containing nanometer-sized particles of magnetite that orient the microbe with the Earth's magnetic fields and allow the organism to seek anaerobic microenvironments. Studying how the microbes synthesize magnetite inside magnetosomes has implications in the fields of evolutionary biology, astrobiology, biotechnology, pharmacology, medicine, and micro-electronics. Oestreicher was nominated for the NSF grant, in part, because of his research on single molecule imaging with EMSL's bio-atomic force microscope. He performed this research in 2007 through an internship with the Summer Research Institute. He co-authored a paper on the team's discovery of a peptide that binds to a metal-oxide surface. This peptide sequence can also be found in multiple copies in two silica-biomineralizing proteins in the cell walls of diatoms.

**Devanathan receives Battelle Community Spirit Award.** EMSL user Ram Devanathan, Pacific Northwest National Laboratory, received the 2008 Battelle Community Spirit Award. A noted materials scientist, he earned this important award for his outstanding efforts in organizing 21 blood drives in 5 years at PNNL. Blood drives provide premature babies, cancer patients, accident victims, people undergoing surgery and others with the blood and blood products they need to survive. As the coordinator, Devanathan and his team scheduled and advertised the quarterly events, set up appointments, and baked refreshments for the donors. "I wanted to give something back to the community," said Devanathan, "And this opportunity to lead the blood drives opened up right after I joined Battelle in 2003."

*Ram Devanathan*

**Beck receives Coast Guard honor.** EMSL researcher Ken Beck received the U.S. Coast Guard Achievement Award for enabling maritime patrols to reliably communicate in the gullies and gorges of the Columbia and Snake rivers. Beck received the award for superior performance of duty while serving as USCG Auxiliary Flotilla 85 Communications Staff Officer from February 2007 to November 2007, in direct support of USCG Aids to Navigation. For 45 years, U.S. Coast Guard patrols have dealt with spotty communications along sections of the Columbia and Snake rivers, especially on 130 miles of the Upper Snake River and 140 miles of the Lake Roosevelt/Spokane River arm. In these areas, steep cliffs block satellite phones, and cell phone reception is intermittent at best and nonexistent at worst. So, patrol teams maintaining the navigational aids for barges and others river traffic may be out of touch with their home base for hours, constituting a dangerous situation. As the newly installed Communications Staff Officer for USCG Flotilla 85, Beck developed and implemented a protocol using a Near Vertical Incident Skywave system, developed in the 1970s. The NVIS system sends high-frequency transmissions into the ionosphere. The signal is reflected and refracted back to earth, creating a circular communication zone with a radius of 25 to 250 miles. Beck designed and assembled the NVIS and extensively field tested the prototype. Further, he modeled the radiofrequency emitted to make sure the field team's exposure was

*Ken Beck received the U.S. Coast Guard Achievement Award for his work on improving communications along troublesome sections of Northwest rivers.*

within permissible environmental exposure limits. The NVIS system that Beck designed is now a model for USCG stations where communications are blocked by the local topography.

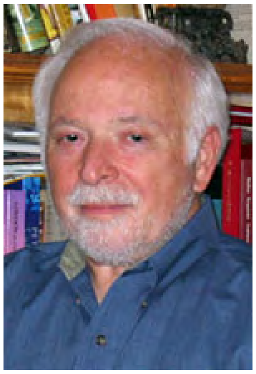
**EMSL Chief Technology Officer, users named AAAS Fellows.** David Koppenaal, EMSL's Chief Technology Officer, and five EMSL users were awarded the distinction of 2007 Fellows of the American Association for the Advancement of Science (AAAS):

- **Koppenaal** was selected for his pioneering development of advanced techniques for analytical mass spectrometry and for distinguished scientific leadership.
- **Ulrike Diebold** of Tulane University was chosen for her pioneering contributions to the surface chemistry and physics of TiO2, particularly to the understanding of the surface structure.
- **Michael F. Hochella, Jr.** of Virginia Tech was awarded for his pioneering contributions to the field of nanogeosciences and microbe-mineral surface interactions, and for outstanding service to the geosciences profession.
- **Samuel Kaplan** of University of Texas-Houston Medical School was honored for his outstanding fundamental research in bacterial photosynthesis and for sustained and effective leadership to the profession of microbiology.
- **Jun Liu** of the Pacific Northwest National Laboratory received the honor for his distinguished contributions to the development, understanding, and commercialization of self-assembled functional nanoporous materials, and to the development of environmentally friendly, solution approaches for oriented nanostructures.
- **Lai-Sheng Wang** of Washington State University was selected for his distinguished and innovative contributions to the field of atomic clusters and for pioneering work on gaseous multiply charged anions.

These researchers are among the 471 members who received the honor for their scientifically or socially distinguished efforts to advance science or its applications. They were honored at the AAAS Annual Meeting in Boston on February 16, 2008.

*Diebold*

*Hochella, Jr.*



*Kaplan*

*Koppenaal*

*Liu*

*Wang*

## *Journal Covers*

During Fiscal Year 2008, research by EMSL users and staff was highlighted on 14 scientific journal covers. The following describe the research that led to these covers.


JMR

Arsenic is an important environmental hazard, but there have been few NMR investigations of its molecular scale structure and dynamics, due principally to the large quadrupole moment of $^{75}$As and consequent large quadrupole couplings. We examine here the potential of existing, single-field solid-state NMR technology to investigate solids containing arsenate and arsenite oxyanions. The results show that current techniques have significant potential for arsenates that do not contain both protonated $H_xAsO_4^{-(3-x)}$ groups and structural water molecules, but that the quadrupole couplings for the arsenites examined here are large enough that interpretation of the spectra is difficult, even at 21.1 T. Compounds that contain both structural $H_2O$ molecules and protonated arsenate groups do not yield resolvable signal, likely a result of $T_2$ effects related to a combination of strong quadrupolar interactions and proton exchange. Spin-echo experiments at 11.7 and 14.1 T were effective for $Li_3AsO_4$ and $CsH_2AsO_4$, as were whole-pattern spikelet experiments for arsenate oxide ($As_2O_5$) at 17.6 and 21.1 T. The central transition resonance of $Ca_3(AsO_4)_2 \cdot 8H_2O$ is ∼6 MHz broad and required a non-conventional, histogram-style spikelet method at high field to improve acquisition efficiency. This approach reduces the acquisition time due to the sensitivity enhancement of the spikelet sequence and a reduction in the number of frequency increments required to map the resonance. Despite the large quadrupole couplings, we have identified a correlation between the $^{75}$As isotropic chemical shift and the electronegativity of the next-nearest neighbor cation in arsenate compounds.

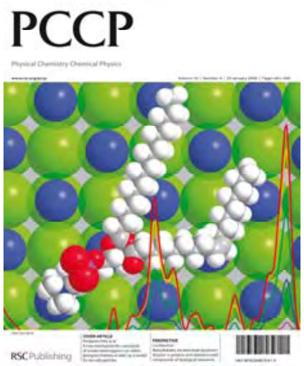
*The research of EMSL users GM Bowers and RJ Kirkpatrick was featured in the October 2007 issue of* Journal of Magnetic Resonance.

Charge loss and desorption kinetics of ions soft-landed onto self-assembled monolayer surfaces. In situ secondary ion mass spectrometry allowed us to explore the kinetics of charge reduction and desorption of different species produced by soft-landing of mass-selected peptide ions onto self-assembled monolayer surfaces (SAM). Soft-landing of doubly protonated ions of Gramicidin S on a fluorinated SAM surface results in the formation of a mixture of doubly protonated, singly protonated, and neutral peptide on the surface. We obtained unique kinetics signatures for all three species retained on the surface and followed their evolution as a function of time. Kinetic modeling demonstrated that charge reduction is responsible for the loss of the doubly protonated ion, while the singly protonated species mainly decays by thermal desorption. Most of the neutral GS molecules are produced by instantaneous charge loss during the collision.

*The research of EMSL users O Hadjar, J Laskin, and JH Futrell was featured in the December 13, 2007, issue of* Journal of Physical Chemistry C.

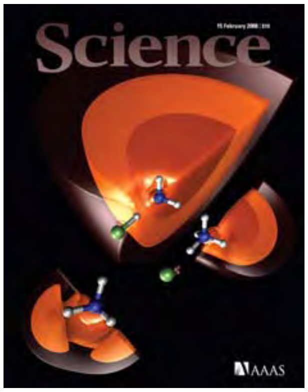
Aromaticity is an important concept in chemistry primarily for organic compounds, but it has been extended to compounds containing transition-metal atoms. Recent findings of aromaticity and antiaromaticity in all-metal clusters have stimulated further research in describing the chemical bonding, structures and stability in transition-metal clusters and compounds on the basis of aromaticity and antiaromaticity, which are reviewed here. The presence of d-orbitals endows much more diverse chemistry, structure and chemical bonding to transition-metal clusters and compounds. One interesting feature is the existence of a new type of aromaticity—δ-aromaticity, in addition to σ- and π-aromaticity which are the only possible types for main-group compounds. Another striking characteristic in the chemical bonding of transition-metal systems is the multi-fold nature of aromaticity, antiaromaticity or even conflicting aromaticity. Separate sets of counting rules have been proposed for cyclic transition-metal systems to account for the three types of σ-, π- and δ-aromaticity/antiaromaticity. The diverse transition-metal clusters and compounds reviewed here indicate that multiple aromaticity and antiaromaticity may be much more common in chemistry than one would anticipate. It is hoped that the current review will stimulate interest in further understanding the structure and bonding, on the basis of aromaticity and antiaromaticity, of other known or unknown transition-metal systems, such as the active sites of enzymes or other biomolecules which contain transition-metal atoms and clusters.

*The research of EMSL users DY Zubarev, BB Averkiev, HJ Zhai, LS Wang, and AI Boldyrev was featured in the January 14, 2008, issue of* Physical Chemistry Chemical Physics (PCCP).



The ozonolysis of an approximately one monolayer film of 1-oleoyl-2-palmitoyl-*sn*-glycero-3-phosphocholine (OPPC) on NaCl was followed in real time using diffuse reflection infrared Fourier transform spectrometry (DRIFTS) at 23 °C. Matrix-assisted laser desorption/ionization (MALDI) mass spectrometry and Auger electron spectroscopy were used to confirm the identification of the products. Ozone concentrations ranged from $1.7 \times 10^{12}$ to $7.0 \times 10^{13}$ molecules $cm^{-3}$ (70 ppb to 2.8 ppm). Upon exposure to $O_3$, there was a loss of C=C accompanied by the formation of a strong band at ~1110 $cm^{-1}$ due to the formation of a stable secondary ozonide (1,2,4-trioxolane, SOZ). The yield of the SOZ was smaller when the reaction was carried out in the presence of water vapor at concentrations corresponding to relative humidities between 2 and 25%. The dependencies of the rate of SOZ formation on the concentrations of ozone and water vapor are consistent with the initial formation of a primary ozonide (1,2,3-trioxolane, POZ) that can react with $O_3$ or $H_2O$ in competition with its thermal decomposition to a Criegee intermediate and aldehyde. Estimates were obtained for the rate constants for the POZ thermal decomposition and for its reactions with $O_3$ and $H_2O$, as well as for the initial reaction of $O_3$ with OPPC. The SOZ decomposed upon photolysis in the actinic region generating aldehydes, carboxylic acids and anhydrides. These studies show that the primary ozonide has a sufficiently long lifetime when formed on a solid substrate that direct reactions with $O_3$ and $H_2O$ can compete with its thermal decomposition. In dry polluted atmospheres, ozone–alkene reactions may lead in part to the formation of stable secondary ozonides whose chemistry, photochemistry and toxicity should be taken into account in models of such regions.

*The research of EMSL users F Karagulian, CW Dilbeck, and BJ Finlayson-Pitts as well as EMSL researcher AS Lea was featured in the January 28, 2008, issue of* Physical Chemistry Chemical Physics (PCCP).

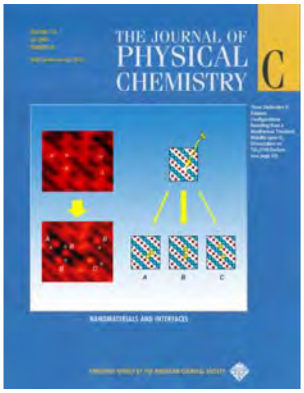


In contrast to widely familiar acid-base behavior in solution, single molecules of $NH_3$ and HCl do not react to form the ionic salt, $NH^+_4Cl^-$, in isolation. We applied anion photoelectron spectroscopy and ab initio theory to investigate the interaction of an excess electron with the hydrogen-bonded complex $NH_3 \cdots HCl$. Our results show that an excess electron induces this complex to form the ionic salt. We propose a mechanism that proceeds through a dipole-bound state to form the negative ion of ionic ammonium chloride, a species that can also be characterized as a deformed Rydberg radical, $NH_4$, polarized by a chloride anion, $Cl^-$.

*The research of EMSL users SN Eustis, D Radisic, KH Bowen, RA Bachorz, M Haranczyk, GK Schenter, and M Gutowski was featured in the February 15, 2008, issue of* Science.

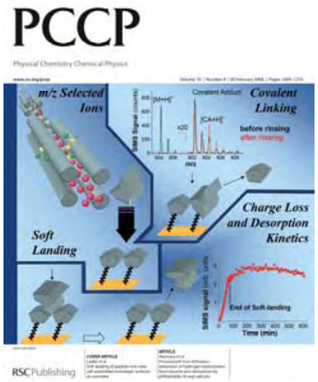
2:1 molar ratio preparation of bismuth with a lipophilic dithiol (3-dimercapto-1-propanol, BAL) significantly reduced extracellular polymeric substances (EPS) expression by *Brevundimonas diminuta* in suspended cultures at levels just below the minimum inhibitory concentration (MIC). Total polysaccharides and proteins secreted by *B. diminuta* decreased by approximately 95% over a 5-day period when exposed to the bismuth-BAL chelate (BisBAL) at near MIC (12 μM). Fourier-transform infrared spectroscopy (FTIR) suggested that a possible mechanism of biofilm disruption by BisBAL is the inhibition of carbohydrate *O*-acetylation. FTIR also revealed extensive homology between EPS samples with and without BisBAL treatment, with proteins, polysaccharides, and peptides varying predominantly only in the amount expressed. EPS secretion decreased following BisBAL treatment as verified by atomic force microscopy and scanning electron microscopy. Without BisBAL treatment, a slime-like EPS matrix secreted by *B. diminuta* resulted in biofouling and inefficient hydrodynamic backwashing of microfiltration membranes.

*The research of EMSL users AR Badireddy, S Chellam, S Yanina, P Gassman, and KM Rosso was featured in the February 15, 2008, issue of* Biotechnology and Bioengineering.



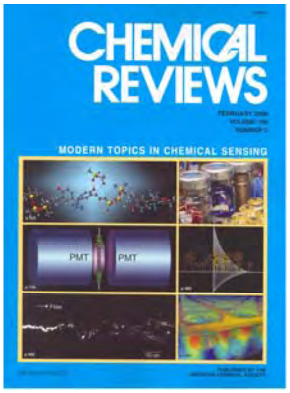
Three distinctive O adatom configurations resulting from a nonthermal, transient mobility upon $O_2$ dissociation on the $TiO_2$(110) surface. Tracking the same region of the reduced $TiO_2$(110) surface by STM before and after oxygen exposure at RT demonstrates that $O_2$ molecules dissociate only at the bridging oxygen vacancies, with one O atom healing a vacancy and the other O atom bonding at the neighboring Ti site as an adatom. The greater part of adatoms (~74%) is separated by one lattice constant along the [001] direction from the original vacancy positions, configuration B, whereas others are separated by two lattice constants (~7%) or bonded at the nearest-neighbor Ti sites (~19%), configurations C and A, respectively. Observed lateral distribution of the oxygen adatoms is attained through a limited nonthermal, transient mobility after $O_2$ dissociation. Following a dissociation, the transient motion of the hyperthermal O adatoms on the $TiO_2$(110) surface is steered along the Ti troughs between the bridging O rows.

*The research of EMSL researchers Y Du and I Lyubinetsky and user Z Dohnalek was featured in the February 21, 2008, issue of* Journal of Physical Chemistry C.



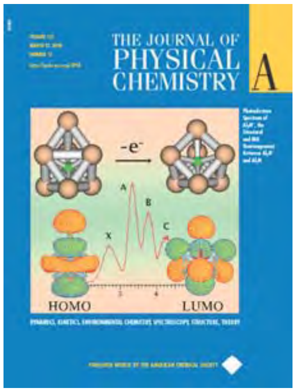
This review is focused on what has been learned in recent research studies concerned with fundamental aspects of soft-landing and reactive landing of peptide ions on self-assembled monolayer surfaces (SAMs). Peptide ions are particularly attractive model systems that provide important insights on the behavior of soft landed proteins, while SAMs provide a convenient and flexible platform for tailoring the interfacial properties of metals and semiconductor surfaces. Deposition of mass-selected ions on surfaces is accompanied by a number of processes including charge reduction, neutralization, covalent and non-covalent binding, and thermal desorption of ions and molecules from the substrate. Factors that affect the competition between these processes are discussed.

*The research of EMSL users J Laskin, P Wang and O Hadjar was featured in the February 28, 2008, issue of* Physical Chemistry Chemical Physics (PCCP).



The development of in situ sensors for ultratrace detection applications in process control and environmental monitoring remains a significant challenge. Such sensors must meet difficult detection limit requirements while selectively detecting the analyte of interest in complex or otherwise challenging sample matrixes. Nowhere are these requirements more daunting than in the field of radionuclide sensing for α- and β-emitting radionuclides in water. The detection limit requirements can be extremely low. Nevertheless, a promising approach to radionuclide sensing based on preconcentrating minicolumn sensors has been developed. In addition, a method of operating such sensors, which we call equilibration-based sensing, has been developed that provides substantial preconcentration and a signal that is proportional to analyte concentration, while eliminating the need for reagents to regenerate the sorbent medium following each measurement. While this equilibration-based sensing method was developed for radionuclide sensing, it can be applied to nonradioactive species as well, given a suitable on-column detection system. By replacing costly sampling and laboratory analysis procedures*, in situ* sensors could have a significant impact on monitoring and long-term stewardship applications.

*The research of EMSL users JW Grate, OB Egorov, MJ O'Hara, and TA DeVol was featured in the February 2008 issue of* Chemical Reviews. In addition, the cover also features a second research project of Jay Grate's, “Hydrogen-Bond Acidic Polymers for Chemical Vapor Sensing.”

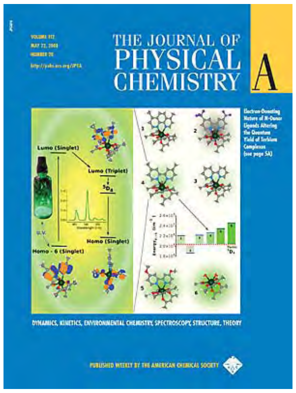


Photoelectron spectrum of $Al_7N^-$, the structural and MO rearrangement between $Al_7N^-$ and $Al_7N$. Photoelectron spectra of $Al_7N^-$ have been obtained at three photon energies. Ab initio vertical electron detachment energies are in excellent agreement with the experimental data. The global minimum structure of $Al_7N^-$ is found to possess $C_{3v}$ symmetry, which can be viewed as an Al atom capping a face of a N-centered $Al_6N$ octahedron.

*The research of EMSL users BB Averkiev, S Call, AI Boldyrev, LM Wang, W Huang, and LS Wang was featured in the March 6, 2008, issue of* Journal of Physical Chemistry A.

A live, in-situ metabolomics capability was developed for prokaryotic cultures under controlled growth conditions. Toward this goal, a radiofrequency-transparent bioreactor was developed and integrated with a commercial wide-bore nuclear magnetic resonance (NMR) imaging spectrometer and a commercial bioreactor controller. Water suppressed $^1H$ NMR spectroscopy was used to monitor glucose and fructose utilization and byproduct excretion by *Eubacterium aggregans* (an anaerobic bacterial species relevant for biofuel production) under controlled batch and continuous culture conditions. The resulting metabolite profiles (short chain organic acids and ethanol) and trends are consistent with existing knowledge of its metabolism. However, our study also showed that *E. aggregans* produces lactate end product in significant concentrations—a result not previously reported. The advantages of live in-situ microbial metabolomics analysis and its complementariness with functional genomics/systems biology methods are discussed.

*The research of EMSL users PD Majors, JS McLean and JCM Scholten was featured in the May 2008 issue of* Journal of Magnetic Resonance.

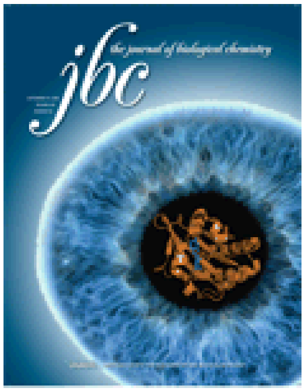


Varying the electron nature of *p,p'*-substituents on the N-donor neutral ligand coordinated to a Tb(III) center leads to changes in the lowest triplet state energy of Tb(III)-acetylacetonates. Consequently, the relative quantum yields of the complexes can be tuned. Experimentally synthesized systems are measured relative to their brightness, whereas theory determines the HOMO-LUMO gap.

*The research of EMSL users CR De Silva, Z Zheng, and LR Corralesw and EMSL researcher J Li was featured in the May 27. 2008, issue of* Journal of Physical Chemistry A.

This article summarizes experimental and theoretical evidence for the existence of four distinct binding modes for complexes of anions with charge-neutral arenes. These include C–H hydrogen bonding and three motifs involving the arene–π system—the noncovalent anion–π interaction, weakly covalent σinteraction, and strongly covalent σ interaction.

*The research of EMSL users BP Hay and VS Bryantsev was featured in the June 7, 2008, issue of* Chemical Communications.



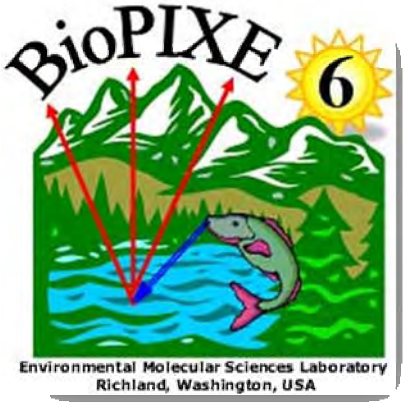
The photoreceptor phosphodiesterase (PDE6) regulates the intracellular levels of the second messenger cGMP in the outer segments of cone and rod photoreceptor cells. PDE6 contains two regulatory GAF domains, of which one (GAF A) binds cGMP and regulates the activity of the PDE6 holoenzyme. To increase our understanding of this allosteric regulation mechanism, we present the 2.6Å crystal structure of the cGMP-bound GAF A domain of chicken cone PDE6. Nucleotide specificity appears to be provided in part by the orientation of Asn-116, which makes two hydrogen bonds to the guanine ring of cGMP but is not strictly conserved among PDE6 isoforms. The isolated PDE6C GAF A domain is monomeric and does not contain sufficient structural determinants to form a homodimer as found in full-length PDE6C. A highly conserved surface patch on GAF A indicates a potential binding site for the inhibitory subunit Pγ. NMR studies reveal that the apo-PDE6C GAF A domain is structured but adopts a significantly altered structural state indicating a large conformational change with rearrangement of secondary structure elements upon cGMP binding. The presented crystal structure will help to define the cGMP-dependent regulation mechanism of the PDE6 holoenzyme and its inhibition through Pγ binding.

*The research of EMSL users SE Martinez, CC Heikaus, RE Klevit, and JA Beavo was featured in the June 7, 2008, issue of* Journal of Biological Chemistry.

# Outreach Activities

The following outreach activities were conducted by EMSL staff in Fiscal Year 2008:

*In June 2008, EMSL launched a new brand and an easier-to-use website.*



*EMSL hosted BioPIXE 6 in June 2008.*

- In June 2008, EMSL rolled out a new brand meant to portray EMSL to our users and stakeholders as DOE's premier national scientific user facility, through five main attributes: Integration, Expertise, Unique Collaborative Environment, State-of-the-Art Instrumentation, and Economical. As part of the brand rollout, EMSL's website was enhanced to make it an easier-to-use tool for users, and highlights, brochures, newsletters, posters, and other outreach tools were developed, and continue to be develop, to help enhance outreach activities.

- In June 2008, EMSL hosted BioPIXE 6**,** a meeting dedicated to advances in biological, medical and environmental applications of proton induced x-ray emission. EMSL staff co-chaired this event with colleagues from the University of California at Davis. More than 50 participants from 31 institutions, many from international universities, attended the workshop.

- In September 2008, EMSL hosted the Pacific Northwest Chapter of AVS Symposium. Nearly 75 faculty members, national laboratory researchers, and regional students attended two days of invited and contributed talks, a poster session, and vendor exhibit, and were given tours of EMSL capabilities.

- EMSL staff organized and hosted the joint Washington State University/University of Washington course, “Nanoclusters, Nanomaterials, and Nanotechnologies,” on May 12-23, 2008. This course involved lectures by EMSL staff and university faculty from both of those universities as well as the University of Idaho. This course was restricted to 10 students to enhance interactions with lecturers and enable the students to perform small projects using EMSL capabilities.

*EMSL Lead Scientist for Interfacial Chemistry, Don Baer (center), with participants of the EMSL-hosted “Nanoclusters, Nanomaterials, and Nanotechnologies” course.*

- EMSL staff led the organization of a topical conference on "*In situ* Microscopy and Spectroscopy: Interfacial and Nanoscale Science" for the American Vacuum Society as part of the 55th International Symposium of the AVS in Boston.

- EMSL staff gave invited talks on the user facility and its capabilities at venues such as Migration ’07, the Environmental Remediation Sciences Program annual meeting, and the Genomes to Life annual meeting.

- In April 2008, EMSL hosted the meeting of the National User Facility Organization, with 40 participants attending from locations such as Lawrence Berkeley National Laboratory’s Advanced Light Source, Oak Ridge National Laboratory’s Center for Nanophase Materials Science, and Argonne National Laboratory’s Advanced Photon Source. EMSL brought in speakers such as Pedro Montano, Director of Scientific User Facilities for the DOE Office of Basic Energy Sciences, who discussed future challenges for Basic Energy Sciences’ user facilities; Linda Horton, Director of the Center for Nanophase Materials Sciences, who discussed the nanoscale science research centers; and Jack Bagley, Battelle Vice President of External Relations, who discussed opportunities and challenges of scientific funding.

- A total of 200 tours were given in EMSL, ranging from local students to high-level political and DOE officials. Stops on the tour include the supercomputer, the NMR lab, laser and surface science capabilities, and the mass spectrometry lab.

### *User Surveys*

In Fiscal Year 2008, EMSL conducted two user surveys to determine satisfaction with availability and performance of facilities and equipment, assistance of technical and administrative staff, training and safety procedures, and the user proposal process.

- In October 2008 (results not yet published), 188 responses (40.9%) were received out of 460 surveys sent out. The responses constituted an 88.9% satisfaction rate.

- In April 2008 (http://www.emsl.pnl.gov/access/surveys/), 371 responses (75.2%) were received out of 493 surveys sent out. The responses constituted an 88.9% satisfaction rate.

Specific comments from users and responses by EMSL to those comments are available at the web addresses listed above.

# Atmospheric Aerosol Chemistry: An Emerging Science Theme

Atmospheric aerosols play an important role in global climate change. Variations of aerosols are recognized as a significant forcing factor that alters the planetary radiation balance onto and away from the Earth, thus contributing to global temperature change. The effects of climate forcing caused by aerosols are not well understood, especially in the case of anthropogenic aerosols. Indeed, the effect of aerosols has been one of the greatest sources of uncertainty in efforts to interpret climate change that occurred in the past century and to project future climate change.

The development of specialized abilities to characterize the overall and surface composition and chemistry of individual particles (or small collections of particles) has led to increased interface and particle analysis activities related to atmospheric aerosol chemistry. Several EMSL users have identified aerosol chemistry as an area that should be of growing scientific importance and impact to understanding local pollution, aspects of climate change, and health effects. This developing area has a range of analysis needs and capability requirements that overlap with aspects of the Science of Interfacial Phenomena science theme, but also move it in new directions.

This emerging science theme is being formulated around the following specific, key scientific topical areas that the aerosol chemistry and atmospheric science communities face today and will continue to face in the future:

- *Developing novel analytical platforms for comprehensive chemical and physical characterization of organic aerosols*
- *Evaluating dynamics of cloud-aerosol interactions and their impacts*
- *Gaining critical knowledge of life cycle and long-term aging of aerosols in the atmospheric environment.*

This science theme is designed to advance the state of knowledge of aerosol physics and chemistry from the molecular level to regional and global scales and their impacts on climate change. State-of-the-art instrumentation at EMSL will be used to characterize the size, composition, density, morphology, chemical reactivity, and cloud interactions of aerosol particles. The research will employ a collaborative and interdisciplinary approach that will combine both the unique analytical capabilities of EMSL and the research expertise of EMSL scientific staff and the user community.

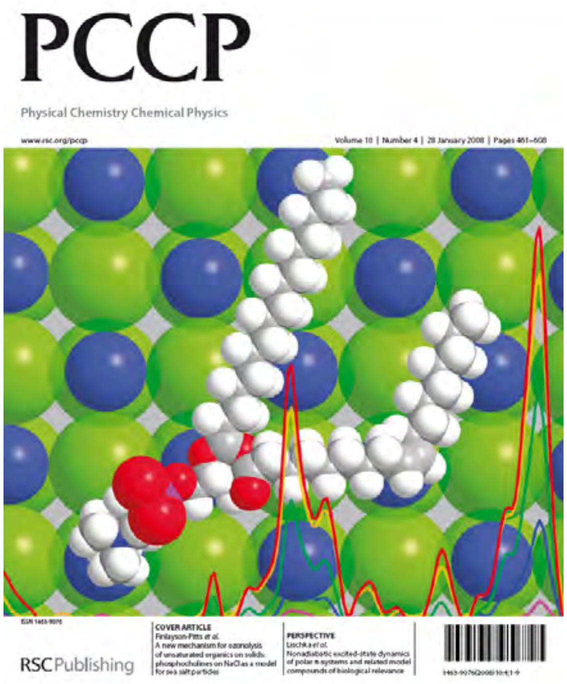
Highlights of research performed in Fiscal Year 2008 under EMSL's emerging Atmospheric Aerosol Chemistry science theme are shown below.

# A New Mechanism for Ozonolysis of Unsaturated Organics on Solids: Phosphocholines on NaCl as a Model for Sea Salt Particles

***F Karagulian[a], AS Lea[b], and BJ Finlayson-Pitts[a]***
*(a) University of California, Irvine, California*
*(b) EMSL, Richland, Washington*

*Distinguished EMSL user Barbara Finlayson-Pitts (University of California, Irvine) collaborated with EMSL researcher Scott Lea to determine the effect of ozone and ultraviolet light exposure on phospholipid coated salt crystals using Fourier transform infrared spectrometry, matrix-assisted laser desorption/ionization mass spectrometry, and Auger electron spectroscopy. They found a new mechanism for the ozonolysis of unsaturated organics on aerosols that may increase the understanding of chemistry, photochemistry, and toxicity of these aerosols in dry, polluted environments.*

Sea salt particles are a major contributor to the global aerosol burden. They are formed by wave action, which carries along organic material with the sea salt. A major source of this organic layer is the decomposition of marine organisms, which have biomembranes that are a mixture of lipids, hydrophobic proteins, and carbohydrates. Phospholipids and fatty acids are common products of biomembrane disintegration. Previous work has indicated that fatty acid lipids in sea salt particles can be enhanced by factors of (5-9)$\times 10^4$ compared to ocean surface water. An organic coating on sea salt particles is expected to modify the chemical and physical properties of the particles.



PCCP

Physical Chemistry Chemical Physics

www.rsc.org/pccp

Volume 10 | Number 4 | 28 January 2008 | Pages 461–608

ISSN 1463-9076

RSC Publishing

COVER ARTICLE
Finlayson-Pitts *et al.*
A new mechanism for ozonolysis of unsaturated organics on solids: phosphocholines on NaCl as a model for sea salt particles

PERSPECTIVE
Lischka *et al.*
Nonadiabatic excited-state dynamics of polar π-systems and related model compounds of biological relevance

***Figure 1.*** *Model of OPPC adsorbed onto NaCl with corresponding DRIFTS spectra upon exposure to ozone superimposed.*

We report on the oxidation of an unsaturated phospholipid, 1-oleoyl-2-palmitoyl-*sn*-glycero-3-phosphocholine (OPPC), adsorbed on NaCl (Figure 1) as a model for lipids on sea salt. The primary ozonide formed in the reaction has a sufficiently long lifetime that it can react with other species such as $O_3$ or $H_2O$. The reaction of OPPC/NaCl with ozone was studied in a flow apparatus equipped with a Fourier transform infrared spectrometer (DRIFTS). $O_3$ and relative humidity were controlled and measured in these experiments. In some experiments, the reacted mixture was photolyzed using a high pressure xenon arc lamp to probe for photochemically active products.

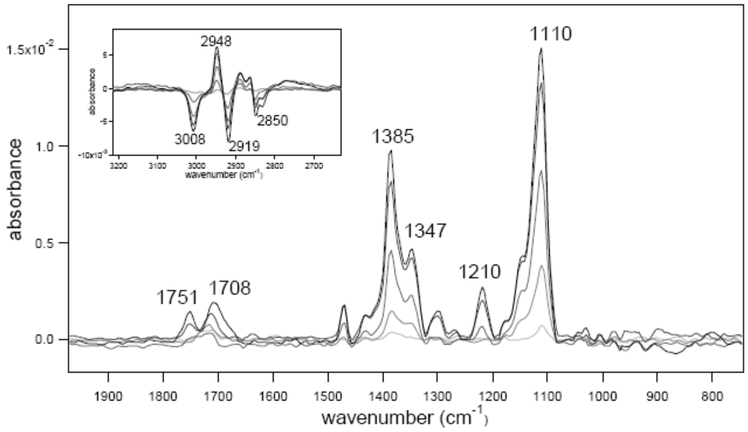


***Figure 2.*** *DRIFTS spectra of OPPC/NaCl upon exposure to 5 × $10^{13}$ $O_3$ $cm^{-3}$ at RH ~ 0%. at increasing ozone exposure times (light gray to black, respectively) of 1, 3, 10, 32 and 56 min.*

Figure 2 shows spectra for OPPC/NaCl during reaction with ozone. A new, strong absorption band is formed at ~1110 $cm^{-1}$ that is characteristic of the peroxide C-O bond of the secondary ozonide ring (SOZ) known to be formed in ozone-alkene reactions. Bands at ~ 1751 $cm^{-1}$ and ~ 1708 $cm^{-1}$ are assigned to carboxylic acids and aldehydes, respectively. It is noteworthy that these bands are much smaller in intensity than the SOZ 1110 $cm^{-1}$ band, despite the fact that their absorption coefficients are larger. This establishes that the SOZ is the major product.

Figure 3 shows the spectra obtained when the reaction was carried out at 2, 10 and 25% RH. There is a dramatic decrease in the SOZ band at 1110 with increasing RH. Changes in SOZ were monitored at an RH of 10% and at $O_3$ concentrations of 7.0 × $10^{13}$ and 1.7 × $10^{12}$ molecule $cm^{-3}$. The relative decrease in SOZ on adding water vapor is more dramatic at the lower ozone concentration, suggesting that the Criegee intermediate (CI) which forms the SOZ can also react with water vapor in competition with SOZ formation. However, even at 10% RH, the water vapor concentration is large so that this reaction competes with other fates of the CI. It should be noted that in separate experiments, addition of water after the reaction had ceased did not change the SOZ peak, showing that it is not the SOZ itself that reacts with water vapor. After photolysis, the elemental composition measured using Auger spectroscopy is similar to that of unreacted OPPC/NaCl. This suggests that during photolysis, volatile products containing oxygen are generated.

These experiments show that the ozone-alkene chemistry on solids is quite different from that in the gas phase or in solution. In particular, the primary ozonide formed on addition of $O_3$ to the double bond is sufficiently stable, with a lifetime of ~100 ms that it can undergo further reactions with $O_3$ and with water vapor. The ozone reaction with OPPC is sufficiently fast that a lifetime of only 15 minutes is expected in the atmosphere at 100 ppb $O_3$. Even at typical concentrations of $O_3$ in remote regions, the OPPC lifetime will still only be on the order of an hour. It is clear from the data that the reaction with $H_2O$ will under most circumstances be the major removal path for the POZ in the atmosphere.

There may be situations where formation of the SOZ represents a significant part of the reaction. For example, consider polluted, dry areas such as Mexico City with $O_3$ peaks of ~400 ppb. Under dry conditions with RH of ~20 %, the lifetime of the POZ is about 90 ms for reaction with $O_3$ and 5 ms for reaction with $H_2O$. While hydrolysis still dominates the removal of POZ, some SOZ would be formed. The health effects of SOZ are not known.

However, given that it is an oxidant and that the organic side chains will increase its solubility in lipids and cell membranes, it has the potential to negatively impact health. This work was featured on the cover of *Physical Chemistry Chemical Physics* in January 2008.

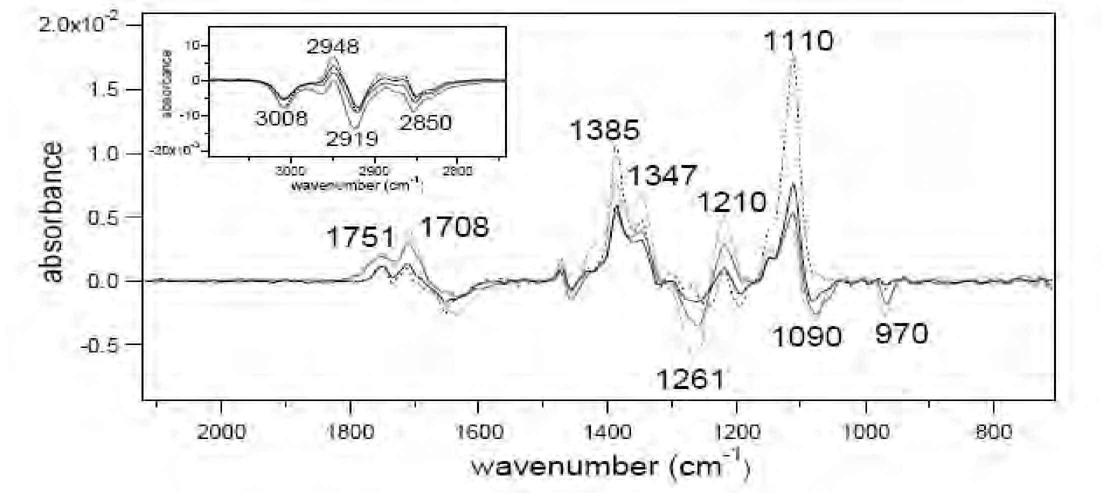


***Figure 3.*** *DRIFTS spectra of OPPC/NaCl upon exposure to 5 × 1013 O3 cm-3 in the presence of water vapor at relative humidities of 2%, 10%, and 25% RH (black to light gray, respectively). The dashed line is the DRIFTS spectrum for a sample reacted with ozone at RH ~ 0%.*

**Citation**

Karagulian F, AS Lea, and BJ Finlayson-Pitts. 2008. "A New Mechanism for Ozonolysis of Unsaturated Organics on Solids: Phosphocholines on NaCl as a Model for Sea Salt Particles." *Physical Chemistry Chemical Physics (PCCP)* 10(4):528-541.

## Experimental Studies of Heterogeneous Gas-to-Particle Reactions Using Novel Particle-on-Substrate Stagnation Flow Reactor Approach

***A Laskin,[(a)] Y Liu,[(a)] H Wang,[(b)] JP Cain,[(b)] VH Grassian,[(c)] and ER Gibson[(c)]***
*(a) EMSL, Richland, Washington*
*(b) University of Southern California, Los Angeles, California*
*(c) University of Iowa, Iowa City, Iowa*

*A novel experimental method for measuring net gas-to-particle reaction probabilities has been developed and applied to a number of reactions relevant to atmospheric aerosol chemistry. Systematic studies focused on definitive and quantitative characterization of nitric acid uptake of NaCl, sea salt and $CaCO_3$ particles under a wide range of relative humidity have been reported using this method.*

A novel Particle-on-Substrate Stagnation Flow Reactor (PS-SFR) experimental approach has been developed by staff and users of EMSL to study the kinetics of heterogeneous, gas-to-sea salt particle reactions. In this new approach, substrate-deposited particles are exposed to reactive gases, followed by chemical analysis of the particles, using advanced instrumentation in EMSL. The reactor design and flow parameters were guided by computational fluid dynamics performed by team members from the University of Southern California to ensure that the diffusion flux was uniform for all particles undergoing reaction. The experimental protocol and data interpretation were successfully implemented in laboratory studies focused on heterogeneous gas-to-particle reactions relevant the atmospheric chemistry of sea salt and mineral dust. A complementary combination of the reported results with previously published single particle mass spectrometry data was essential to understanding uptake kinetics over a wide range of particle sizes and experimental conditions. The developed experimental approach offers options for multi-instrumental analyses of particle samples and therefore can be applicable to a wide variety of reactions of interest not only for the atmospheric chemistry community but also for the surface science and catalysis communities.

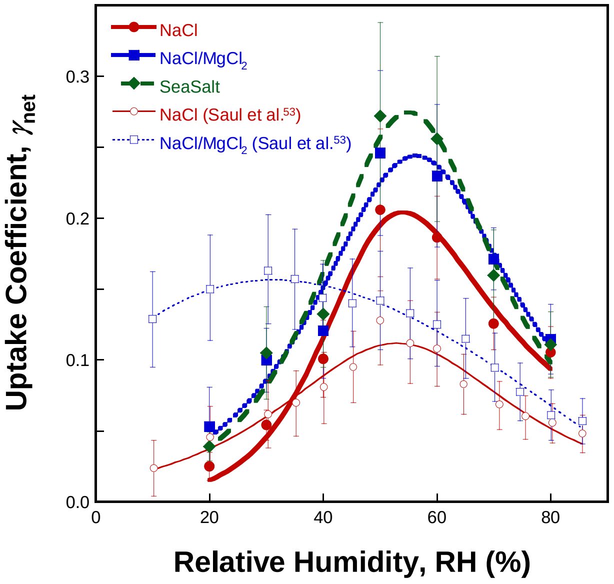


***Figure 1.*** *Values of uptake coefficient as a function of relative humidity for $HNO_3$ reaction with an NaCl, mixture of $NaCl/MgCl_2$ and sea salt particles (Liu et al, 2007).*

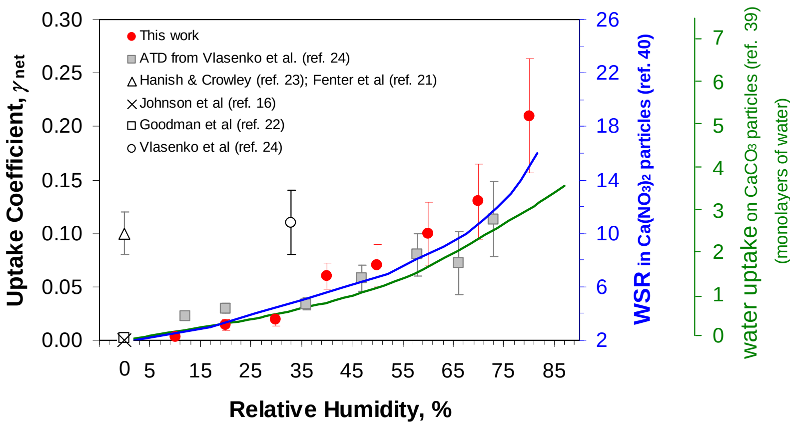


***Figure 2.*** *Experimentally determined uptake coefficient as a function of the relative humidity for $HNO_3$ reaction with $CaCO_3$ particles (Liu et al. 2008).*

Heterogeneous reactions between nitric acid and aerosol particles, such as sea salt and carbonates present in mineral dust, serve as major sinks for gaseous metric acid and nitrogen oxides, which impact the overall chemical balance of the troposphere. Results from our studies using the PS-SFR approach show that NaCl and $CaCO_3$ have a similar reactive $HNO_3$ uptake at RH<40% but exhibits a very different humidity dependence.

The uptake of $HNO_3$ onto NaCl was found to increase with the decreasing RH and peak around a relative humidity of 55%, and then below the efflorescence relative humidity (~45% RH) the uptake coefficient decreases rapidly (Figure 1). While uptake of $HNO_3$ onto $CaCO_3$ was found to increase monotonically with an increase in relative humidity due to hygroscopic growth of the reaction product $Ca(NO_3)_2$ (Figure 2). As a result, if $CaCO_3$ and NaCl aerosol particles are present in the same $HNO_3$ polluted air mass, both heterogeneous reaction channels could occur. They may take place equivalently or competitively, depending on specific conditions. Sea salt and mineral dust particles are the largest components, by mass, of global aerosol burden and contribute substantially to atmospheric chemistry, air quality, and climate change issues.

The developed approach is expected to be applicable to a variety of reactions of interest not only for the atmospheric research community but also for the surface science and catalysis communities. Details of this research have been recently published in the *Journal of Physical Chemistry A*.

**Citations**

Liu Y, JP Cain, H Wang, and A Laskin. 2007. "Kinetic Study of Heterogeneous Reaction of Deliquesced NaCl Particles with Gaseous $HNO_3$ Using Particle-on-Substrate Stagnation Flow Reactor Approach." *Journal of Physical Chemistry A* 111(40):10026-10043.

Liu Y, ER Gibson, JP Cain, H Wang, VH Grassian, and A Laskin. 2008. "Kinetics of Heterogeneous Reaction of $CaCO_3$ Particles with Gaseous $HNO_3$ over a Wide Range of Humidity." *Journal of Physical Chemistry A* 112(7):1561-1571.

## Heterogeneous Reaction of Deliquesced NaCl Particles with Gaseous $HNO_3$

***Y. Liu,[(a)] JP Cain,[(b)] H Wang,[(b)] and A Laskin[(a)]***
*(a) EMSL, Richland, Washington*
*(b) University of Southern California, Los Angeles, California*

*Reactions on atmospheric aerosol particles are known to impact atmospheric composition and chemistry, global radiative forcing and climate change, sky visibility, and public health. Understanding these processes is crucial for our ability to control and predict their effects on the environment.*

Over the last few decades, a great deal of attention has been placed on the fundamental kinetics and mechanism of atmospheric heterogeneous reactions. Reactions involving aerosols are known to impact atmospheric composition and chemistry, global radiative forcing and climate change, sky visibility, and public health. Sea salt aerosols, generated by wind-induced wave action and bubble bursting of seawater, are the second largest component (by mass) of global aerosol burden. These aerosols may undergo heterogeneous reactions with trace species in the atmosphere, including OH, $HNO_3$, $O_3$, $NO_2$, $N_2O_5$, and $ClONO_2$. The net result is that inert halides may be converted to photochemically reactive halogen species, which lead to the production of reactive halogen species upon exposure to sunlight. There has been increasing evidence from laboratory and field studies that these halogen atoms play pivotal roles in the chemistry of the marine boundary layer. For these reasons, a quantitative understanding of the uptake and kinetics of reactive gases on sea salt particles is critical toward elucidating the overall halogen budget and tropospheric chemistry. Figure 1 shows a schematic of a mechanism to create halogens.

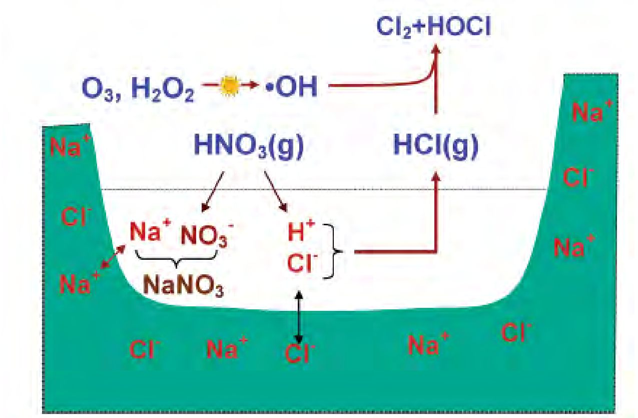


***Figure 1.*** *Heterogeneous reactions occurring in the marine boundary layer: uptake of $HNO_3$ onto NaCl and reaction of its product, HCl, with OH.*

In this work, the authors report on the heterogeneous reaction kinetics of gaseous nitric acid with deliquesced sodium chloride particles, NaCl(aq)+ $HNO_3$(g), to form aqueous sodium nitrate and gaseous hydrochloric acid, $NaNO_3$(aq) + HCl(g), using a novel particle-on-substrate stagnation flow reactor (PS-SFR). This instrument allows the reactions to be studied under conditions, including particle size, relative humidity, and reaction time, directly relevant to the atmospheric chemistry of sea salt particles. Particles deposited onto an electron microscopy grid substrate were exposed to the reacting gas at atmospheric pressure and room temperature by impingement via a stagnation flow inside the reactor. The reactor design and choice of flow parameters were guided by computational fluid dynamics to ensure uniformity of the diffusion flux to all particles undergoing reaction. The reaction kinetics were followed by observing chloride depletion in the particles by computer-controlled scanning electron microscopy with energy-dispersive x-ray analysis (CCSEM/EDX).

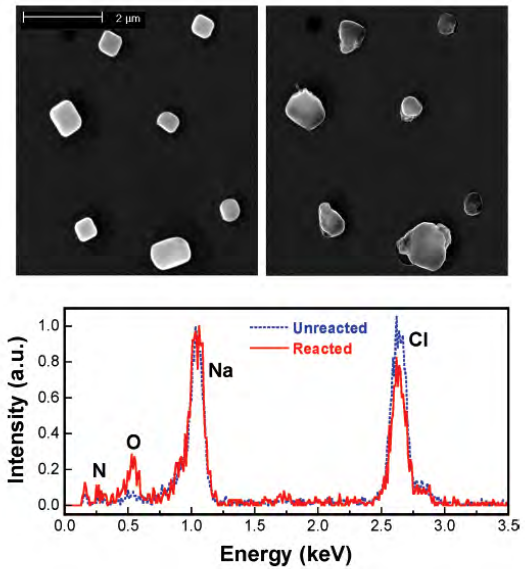


***Figure 2.*** *Top panels: Scanning electron microscope images of NaCl particles before (left) and after (right) reaction with gaseous $HNO_3$ of 6 ppb concentration, 80% relative humidity and reaction time of 210 min. Bottom panel: Typical* energy-dispersive x-ray analysis *spectra of individual NaCl particle before and after reaction.*

Figure 2 shows a scanning electron microscope image of NaCl particles before and after exposure to $HNO_3$. A series of experiments was conducted in which the particle loading, free stream $HNO_3$ concentration, reaction time, particle size, and relative humidity were varied for one or more types of salt particles. Results show that the variation of the apparent, pseudo-first-order rate constant with particle loading and $HNO_3$ concentration in the free stream is entirely consistent with a diffusion-kinetic analysis.

The authors note that micron-size sea salt particles are ubiquitous in and near the marine boundary layer. These particles are responsible for a large fraction of light scattering and backscattering. However, the particles are too large to be efficiently transmitted to single-particle mass spectrometers (SPMS) commonly used to detect chloride depletion. In addition, the fact that the particles must be suspended in a gas requires the reaction to take place in a flow reactor for no longer than tens of seconds, far shorter than the lifetime of typical sea salt particles in atmospheric chemistry. For these reasons, reactions of micron-size particles are not "accessible" by FR-SPMS. However, the PS-SFR experiment coupled with the CCSEM/EDX technique adopted here allows the particles to undergo exposure to a reactive gas over a considerably longer period and is well suited for particles of micron size. The technique also offers options for multi-instrumental microanalysis and is applicable to both laboratory-generated and field-collected samples. It should be noted that this approach does have one important limitation: particles smaller than 0.5 microns may not be accurately probed because of the potential damage caused from the electron beam. These considerations lead the authors to believe that a combination of FR-SPMS and PS-SFR/CCSEM/EDX would be essential to understand uptake over a wide range of particle sizes and experimental conditions. Details of this exciting research have been published as a feature article in the *Journal of Physical Chemistry A*.

**Citation**

Liu Y, JP Cain, H Wang and A Laskin. 2007. "Kinetic Study of Heterogeneous Reaction of Deliquesced NaCl Particles with Gaseous $HNO_3$ using Particle-on-Substrate Stagnation Flow Reactor Approach." *Journal of Physical Chemistry A* 111(40):10026-10043.

## Laboratory Studies on the Effect of Primary Organic Aerosols on Secondary Organic Aerosol Formation

***ML Alexander,[(a)] C Song,[(b)] RA Zaveri,[(b)] JA Thornton,[(c)] A Zelenyuk,[(b)] XY Yu,[(b)] S Madronich,[(d)] and D Maughan[(b)]***

*(a) EMSL, Richland, Washington*
*(b) Pacific Northwest National Laboratory, Richland, Washington*
*(c) University of Washington, Seattle, Washington*
*(d) National Center for Atmospheric Research, Boulder, Colorado*

*The effect of existing primary organic aerosols (POA), typical of automobile and truck emissions, on the formation of secondary organic aerosol (SOA) is investigated in a controlled laboratory setting. The results of these studies showed no enhancement of SOA yields by POA, in sharp contrast to assumptions inherent in current atmospheric models for SOA production, pointing to a need for more sophisticated understanding of the chemical and physical processes underlying SOA formation in the atmosphere.*

A suite of EMSL instrumentation was used in fundamental laboratory studies to evaluate the effect of primary organic aerosol (POA) on secondary organic aerosol (SOA) yields in a laboratory-based smog chamber. The EMSL proton transfer reaction mass spectrometer was used to measure the gas-phase concentrations of $\alpha$-pinene and reaction products resulting from ozonolysis. Particle number concentrations were monitored with a standard scanning mobility particle size, while real-time size, composition and mass concentration were monitored with the EMSL time-of-flight aerosol mass spectrometer. Density of $\alpha$-pinene SOA particles was measured in independent experiments using the EMSL single-particle laser-ablation time-of-flight mass spectrometer. Dioctylphthalate (DOP) and lubricating oil were used as surrogate POA seed aerosols, and oxidation of $\alpha$-pinene by ozonolysis was used as a controlled SOA formation mechanism. All measurements were made in an indoor 8 $m^3$ Teflon smog chamber at PNNL.

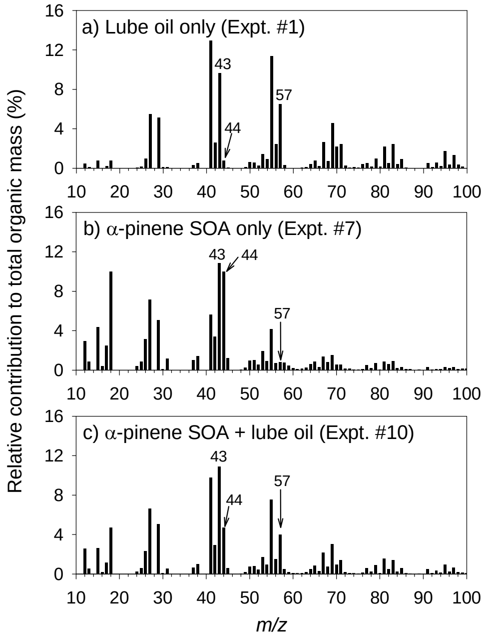


***Figure 1.*** *Representative normalized AMS spectra for (a) lubricating oil,(b) $\alpha$--pinene and (c) $\alpha$--pinene with lubricating oil (Song et al 2007).*

Representative aerosol mass spectra from lubricating oil, pure $\alpha$-pinene SOA particles, and $\alpha$-pinene SOA formed with lubricating oil particles present are shown in Figure 1. These spectra can be qualitatively interpreted using the ratio of molecular fragments at m/Z 57 $(C_4H_9^+)$ to 44 $(CO_2^+)$ to indicate the ratio of hydrocarbon-like aerosol (HOA) to oxygenated organic aerosols (OOA). As expected, the ratio is much higher, 8.9 for lubricating oil than for the more highly oxidized $\alpha$-pinene SOA. The third mass spectrum is for the mixture of lubricating oil and $\alpha$-pinene and is a nominal value. Figure 2 shows the time evolution of the ratio HOA /OOA derived from a statistical analysis of the time-resolved aerosol mass spectra as SOA is formed from ozonolysis.

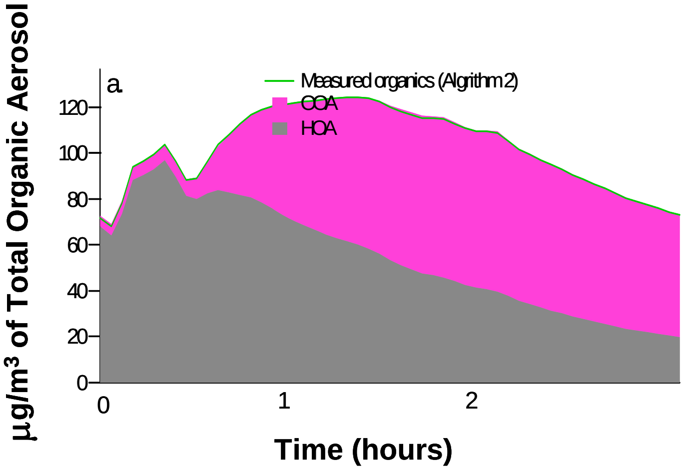


***Figure 2***. *Time evolution of POA and SOA fractions during oxidation of $\alpha$--pinene in the presence of lubricating oil seed.*

Figure 3 (symbols) shows a plot of observed SOA mass for the entire study with no seed, lube oil seed and with DOP seed. The SOA yield *(Y)* is defined as $Y =$ $\Delta$[α-pinene ], where $M_{SOA}$ (μg $m^{-3}$) is the mass concentration of SOA formed and Δ[α-pinene] (μg $m^{-3}$) is the amount of α-pinene reacted with ozone. Also shown are the results of the two-product, semi-empirical Odum model equation, currently the basis for atmospheric SOA models (e.g., Chung and Seinfeld 2002) in the absence of any seed aerosols.

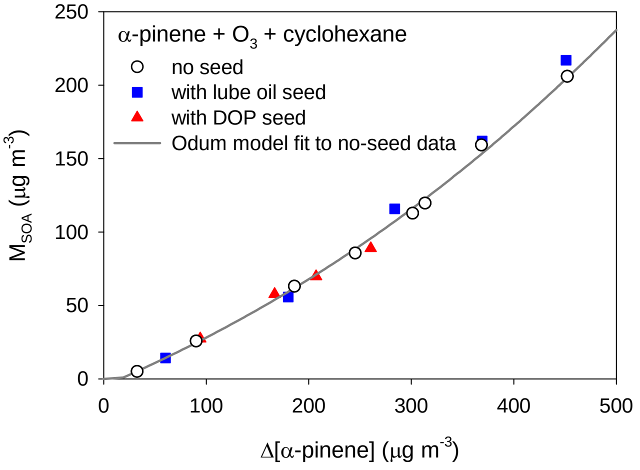


***Figure 3.*** *Comparison of SOA mass produced in the absence and presence of DOP and lubricating oil seed aerosols as a function of amount of α--pinene reacted with fit from Odom model. (Song et al 2007)*

Note that all the $M_{SOA}$ observations for these studies fall on the same baseline curve that was obtained for the unseeded experiments. These results indicate that in the presence of DOP and lubricating oil seed, aerosols do not enhance the formation of SOA mass by providing additional absorbing mass. It therefore appears that the condensed SOA species form a separate organic phase, which then behaves in the same manner as the homogeneously nucleated SOA with regard to the gas-particle partitioning coefficients. Current atmospheric SOA models, based on these results, may erroneously predict high SOA yields. If these results apply to other SOA precursors, the current under-prediction of SOA by current atmospheric models compared to field measurements is more severe than previously believed. This conclusion underscores the need for molecular-level laboratory studies to fully understand the actual chemical and physical processes for SOA formation in the ambient atmosphere at urban, regional, and global scales.

Details of this research were recently published in *Geophysical Research Letters.*

## Citations

Song C, RA Zaveri, ML Alexander, JA Thornton, S Madronich, JV Ortega, A Zelenyuk, XY Yu, A Laskin, and DA Maughan. 2007. "Effect of Hydrophobic Primary Organic Aerosols on Secondary Organic Aerosol Formation from Ozonolysis of α–pinene." *Geophysical Research Letters* 34*:* L20803, doi:10.1029/2007GL030720.

Chung SH, and JH Seinfeld. 2002. "Global Distribution and Climate Forcing of Carbonaceous Aerosols." *Journal of Geophysical Research 107*(D19):4407, doi:10.1029/2001JD001397.

# Application of Methods of High-Resolution Mass Spectrometry to Study Chemistry of Secondary Organic Aerosol

***S Nizkorodov,[(a)] ML Walser,[(a)] AP Bateman,[(a)] A Laskin,[(b)] J Laskin,[(c)] and Y Desyaterik [(c)]***

*(a) University of California, Irvine, California*
*(b) EMSL, Richland, Washington*
*(c) Pacific Northwest National Laboratory, Richland, Washington*

*Methods of high-resolution mass spectrometry have been applied to study chemical composition of secondary organic aerosol (SOA) formed from the ozone-initiated oxidation of limonene. A significantly more complex SOA composition than that predicted by previously reported mechanisms was discovered. A possible reaction mechanism for the formation of the first-generation SOA molecular components has been presented.*

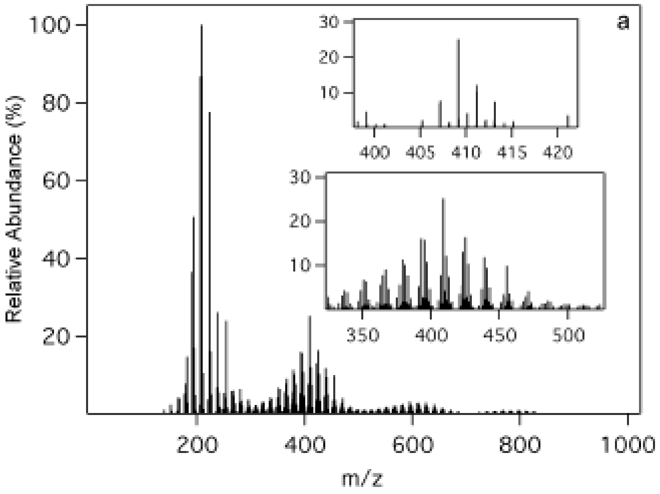


***Figure 1.*** *Representative positive ESI mass spectra of SOA particles extracted in acetonitrile. The data include peaks with >0.5% abundance relative to the largest peak in the spectrum. (Walser et al., 2008).*

High-resolution mass spectrometric characterization of SOA particles formed from the ozone-induced oxidation of limonene revealed that the chemical composition of these particles is significantly more complex than that predicted by the basic Criegee mechanism of alkene ozonolysis. The mass spectra reveal ~1500 condensed products of oxidation, as illustrated in Figure 1. This work convincingly demonstrated that in order to account for the very large number of poly-functional species that exist in SOA in both monomeric and polymeric form, one has to include rich chemistry involving alkylperoxy and alkoxy radicals formed from the decomposition of carbonyl oxide intermediates. The authors described a minimal set of reactions required to produce a distribution of limonene ozonation products that is consistent with mass spectrometric observations. Even with a fairly restrictive set of reaction rules, inclusion of alkylperoxy and alkoxy chemistry in limonene ozonation produces some 1000 products with 140 unique m/z values in the monomeric mass range (m/z <300). The discussed mechanism includes known isomerization and addition reactions of the carbonyl oxide intermediates generated during the ozonation of limonene. In addition, it includes isomerization and decomposition pathways for alkoxy radicals resulting from unimolecular decomposition of carbonyl oxides that have been disregarded by previous studies. The isomerization reactions yield numerous products with a progressively increasing number of alcohol and carbonyl groups, whereas C–C bond scission reactions in alkoxy radicals shorten the carbon chain. Together these reactions yield a large number of isomeric products with broadly distributed masses. A qualitative agreement is found between the number and degree of oxidation of the predicted and measured reaction products in the monomer product range.

The large number of isomeric products produced in the oxidation of just one terpene shows how challenging it will be to obtain detailed characterization of molecular composition of ambient SOA particles that typically result from oxidation of multiple precursors. The ultimate goal of research on chemical mechanisms of SOA formation is to find out which reactions out of the infinite number of possibilities actually take place, and which are likely to be insignificant. It is expected that for such complex systems, the answer to this question will come from coupling mass spectrometry and information theory, and this work can be viewed as the first step in that direction.

Details of this research were recently published in *Physical Chemistry Chemical Physics.*

**Citation**

Walser ML, Y Desyaterik, J Laskin, A Laskin, and SA Nizkorodov. 2008. "High-Resolution Mass Spectrometric Analysis of Secondary Organic Aerosol Produced by Ozonation of Limonene" *Physical Chemistry Chemical Physics* 10(7):1009-1022.

## Chemical Speciation of Sulfur in Marine Particles

***RJ Hopkins,[a] Y Desyaterik,[b] AV Tivanski,[a] RA Zaveri,[b] CM Berkowitz,[b] T Tyliszczak,[a] MK Gilles,[a] and A Laskin[c]***

*(a)* *Lawrence Berkeley National Laboratory, Berkeley, California*
*(b)* *Pacific Northwest National Laboratory, Richland, Washington*
*(c)* *EMSL, Richland, Washington*

*Detailed chemical speciation of field-collected particles from the marine boundary layer over the California current was performed using a combination of complementary microanalysis techniques. On the basis of composition, morphology, and chemical bonding information, two externally mixed, distinct classes of sulfur-containing particles were identified: chemically modified (aged) sea salt particles and secondary-formed sulfate particles. The results indicate substantial heterogeneous replacement of chloride by methanesulfonate* ($CH_3SO_3^-$) *and non-sea-salt sulfate* (nss-$SO_4^{2-}$) *in sea-salt particles with characteristic ratios of nss-S/Na* $> 0.10$ *and* $CH_3SO_3^-$/nss-$SO_4^{2-} > 0.6$.

A research team of EMSL staff and users presented the first observations of both $CH_3SO_3^-$ and $SO_4^{2-}$ sulfur compounds in marine aerosol, identified on a single-particle basis. Both time-of-flight-secondary ion mass spectrometry (TOF-SIMS) and scanning transmission x-ray microscopy/near-edge x-ray absorption fine structure techniques (STXM/NEXAFS) indicate an external mixture consisting primarily of two particle classes: mixed sea salt/$CH_3SO_3^-$/$SO_4^{2-}$ and S-rich particles of mixed $H_2SO_4$/$(NH_4)_2SO_4$ composition ( Figure 1). Unambiguous, qualitative speciation of sulfur-containing compounds and quantitative assessment of the $CH_3SO_3^-$/nss-$SO_4^{2-}$ ratios have been facilitated using combined data sets from three techniques: (1) computer-controlled scanning electron microscopy/energy-dispersed X-ray analysis, quantitative assessment of elemental composition of individual particles; (2) TOF-SIMS, qualitative molecular speciation of sulfur-containing compounds in individual particles; and (3) STXM/NEXAFS, quantitative assessment of different forms of sulfur within individual particles. The data provided by these techniques offer a rich set of qualitative and quantitative information that is of primary importance to atmospheric chemistry processes in the marine boundary layer involving sea-salt and marine sulfate particles.

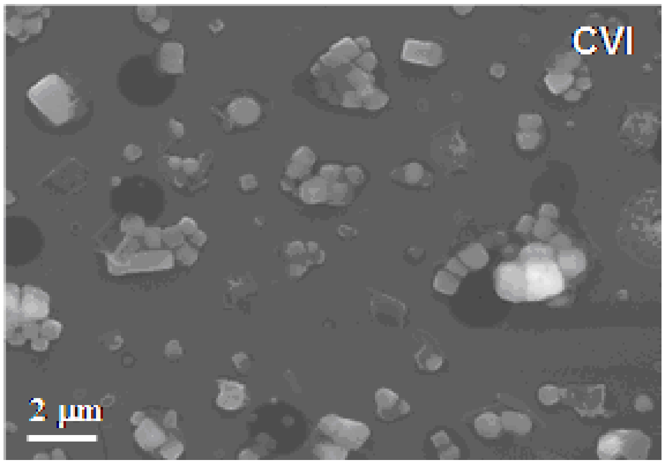


***Figure 1.*** *Scanning electron microscopy image of marine particles. Sea-salt particles are larger, irregularly shaped supermicron particles with NaCl cubic crystal cores. Ammonium sulfate particles are spherical submicron particles (Hopkins et al., 2008).*

For the first time, size-dependent nss-S/Na and $CH_3SO_3^-$/nss-$SO_4^{2-}$ ratios are reported for marine particles. Characteristic ratios of nss-S/Na > 0.10 are reported for sea-salt particles, with higher values observed for smaller particles, indicating more extensive formation of sulfur-containing salts. Characteristic ratios of $CH_3SO_3^-$/nss- $SO_4^{2-}$ > 0.60 are reported for sea-salt particles of all sizes, with higher values for large particles (Figure 2). This indicates that $CH_3SO_3^-$ salts are likely the dominant form of nss-sulfur in large particles, while nss- $SO_4^{2-}$ is more common in smaller particles. In the past, much attention has been given to the hygroscopic and optical properties of sea-salt aerosols and the corresponding mixed sea salt/sulfate particles that can be formed as a result of the DMS $\rightarrow SO_2 \rightarrow H_2SO_4$ reaction sequence that is assumed to dominate in the mid latitude marine boundary layer. However, our analysis of field-collected sea-salt particles indicate that DMS conversion to

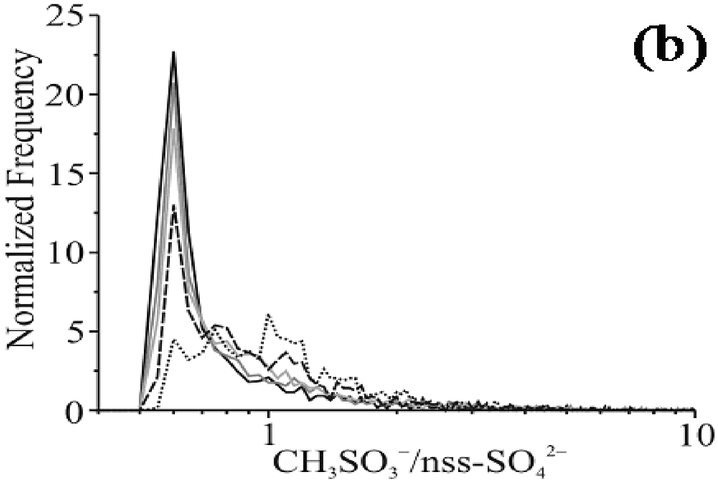


***Figure 2.*** *Distribution of $CH_3SO_3^-$ to nss-$SO_4^{2-}$ ratio present in particles with diameter in the range 0.31 – 0.5, 0.5 – 0.79, 0.79 – 1.26, 1.26 – 2 and > 2 μm (black, dark grey, light grey, dashed and dotted lines, respectively). (Hopkins et al., 2008).*

MSA can result in $CH_3SO_3^-$/nss- $SO_4^{2-}$ > 0.60 and nss-S/Na > 0.1 ratios, as were observed under specific conditions of the coastal area north of San Francisco. These findings indicate that modeling of the marine boundary layer aerosols and cloud formation processes require extensive data on the hygroscopic and CCN properties of mixed sea salt/$CH_3SO_3^-$/$SO_4^{2-}$ and perhaps other organo-sulfur particles. These data are fairly scarce and require future research.

Details of this research were recently published in the *Journal of Geophysical Research – Atmospheres*

**Citation**

Hopkins RJ, Y Desyaterik, AV Tivanski, RA Zaveri, CM Berkowitz, T Tyliszczak, MK Gilles, and A Laskin. 2008. "Chemical Speciation of Sulfur in Marine Cloud Droplets and Particles: Analysis of Individual Particles from the Marine Boundary Layer over the California Current." *Journal of Geophysical Research D – Atmospheres* 113:D04209, doi:10.1029/2007JD008954.

# Biological Interactions and Dynamics

Understanding and optimizing the response of biological systems to their environment can have a significant impact on achieving viable solutions to several problems of national concern. For example, a deep knowledge of anaerobic microbial metabolism can improve national efforts in environmental cleanup and site stewardship, and help provide clean and secure energy. Molecular-level measurements and insights into biochemical processes are also foundational to building predictive computational models that would improve our ability to use microbes effectively and safely as an approach to mitigate the impacts of energy-production activities on the environment and human health and to extend basic scientific research.

Recent advances in whole-genome sequencing of a variety of organisms and improvements in high-throughput instrumentation have contributed to a rapid transition of the biological research paradigm towards understanding biology at a systems level. As a result, biology is evolving from a descriptive to a quantitative, ultimately predictive science where the ability to collect and productively use large amounts of biological data is crucial. Understanding how the ensemble of proteins in cells gives rise to biological outcomes is fundamental to systems biology. Advances in systems-level research will require new technologies and approaches to measure and track the temporal and spatial disposition of proteins in cells and how protein complexes give rise to specific activities.

To help facilitate the transition of biology to a more quantitative science, EMSL encourages user proposals with a focus on the following key topical areas:

- *Understanding the protein and metabolite composition of cells as well as the activities, structures and chemical modifications of individual proteins and protein complexes.*
- *The dynamics of cellular protein composition and well as the localization and assembly of multiprotein complexes.*
- *The properties and dynamics of biological membranes*
- *The interaction of cells with each other and with the extracellular environment.*

Work in these topical areas can utilize current EMSL capabilities as well as extend capabilities into new technical areas. For example, a full understanding of the structure, function, and dynamics of multi-protein complexes and a detailed metabolite profiling of many cells will require extending current EMSL capabilities in high-throughput mass spectrometry and NMR. Work is currently underway to enhance EMSL capabilities in the analysis of microbial membranes and cellular interactions by the development of new techniques, such as cryo-TEM, and multimodal and multispectral microscopy. Efforts are also underway to integrate and analyze the large amounts of data generated by EMSL instruments through an integrated data management system. Proposals to use these developing capabilities are particularly encouraged.

Highlights of research performed in Fiscal Year 2008 under EMSL's Biological Interactions and Dynamics science theme are shown below.

# Submicrometer and Nanoscale Inorganic Particles Exploit the Actin Machinery to be Propelled Along Microvilli into Alveolar Cells

**G Orr,[a] DJ Panther,[a] JL Phillips,[a] BJ Tarasevich,[a] A Dohnalkova,[b] D Hu,[a] JG Teeguarden,[a] and JG Pounds[a]**

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

*The explosion in micro- and nanotechnology is expected to increase our exposure to submicrometer and nanoscale particles, but the impact of this exposure on human health is unclear. Since the cellular interactions and pathways of the particles are going to drive cellular response and ultimately the level of toxicity, we have been studying these cellular processes while focusing on well-defined particles and delineating relationships between particle properties and potential toxicity or biocompatibility.*

The environmental or occupational exposure to submicrometer and nanoscale materials is expected to increase within the next few years as the result of their increased use in industrial and medical applications. When inhaled, these particles are likely to reach the alveoli, where alveolar type II epithelial cells are found. These cells, which are distinguished by apical microvilli, play critical roles in the function of the alveoli and participate in the immune response to certain particles and pathogens by releasing chemokines. However, the cellular interactions of the particles, which drive the cellular responses, are still unclear. Adverse effects of nanoparticles have been attributed, in part, to the unique

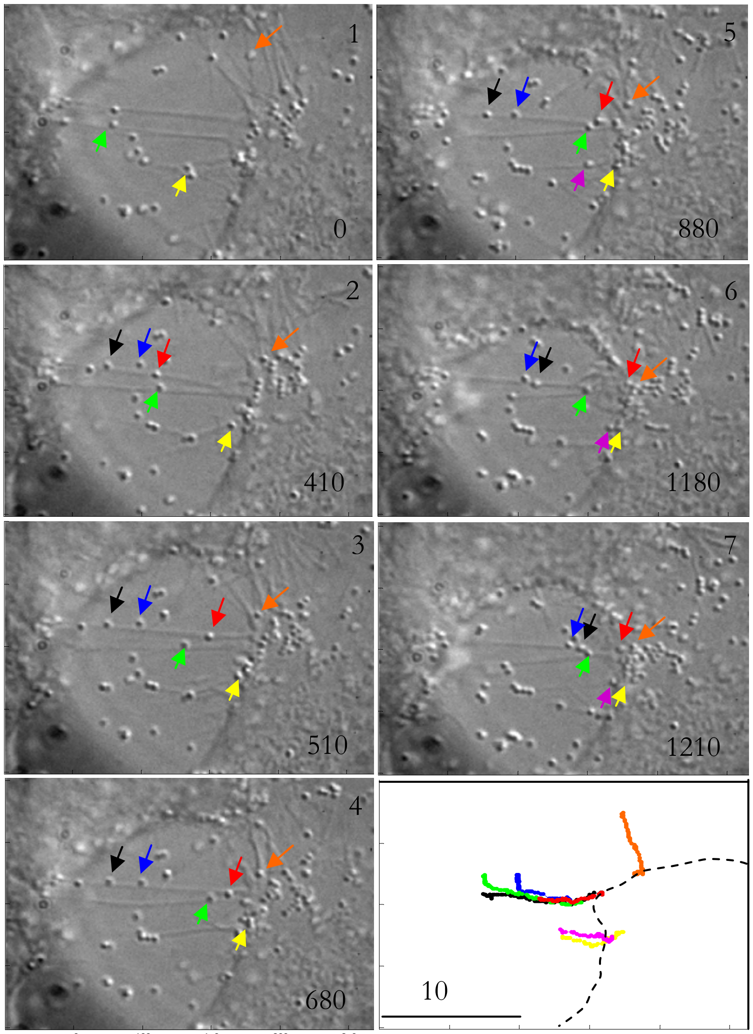


***Figure 1.*** *The retrograde motion unravels the coupling of the particles with the intracellular environment across the cell membrane.*

properties of materials at the nanoscale. However, little is known about the cellular interactions of individual or small nanoparticle aggregates, mostly because of their tendency to agglomerate under experimental conditions.

Since the cellular interactions and internalization pathways of inhaled particles are going to drive the cellular response and ultimately the impact on the pulmonary system, we investigated the surface-dependent interaction of individual or small aggregates of submicrometer and nanoscale particles, as they are likely to be presented to cells *in vivo*. Using differential interference contrast (DIC) and total internal reflection fluorescence (TIRF) microscopy at 200 times magnification, we find that positively charged 100-nm and 500-nm precipitated amorphous silica particles can travel along microvilli toward the cell body. The retrograde motion unravels the coupling of the particles with the intracellular environment across the cell membrane. Figure 1 demonstrates the retrograde motion of positively charged 500-nm particles, using a time series of DIC images that were acquired at 10-second intervals. Each particle is followed along the sequence of the images with a color-coded arrow that is added when the particle lands on the cell. Particles can dwell in their landing spot before starting to move, or become engaged in the motion immediately after landing. By the end of the series, the particles are found by the cell body where other particles are already accumulated.

Figure 2 demonstrates the retrograde motion of 100-nm particles using single-molecule fluorescence techniques. The images in Figure 2a were selected from a time series that was acquired using TIRF microscopy at 10-second intervals. The fluorescent spot that is indicated by the arrow in the first image is estimated to represent one nanoparticle or a cluster containing two nanoparticles. The estimation is based on the intensity of the fluorescent spot and on the size of the spot, which is near the diffraction limit of the light (3 x 3 pixels). The particle travels along a microvillus that originates from the apical surface of the cell body, as shown in Figure 2b where the trajectory of the nanoparticle is overlaid on the DIC image. Interestingly, the motion pattern of the nanoparticle, although clearly directed toward the cell body, includes both rearward and forward motions, as demonstrated in the trajectory.

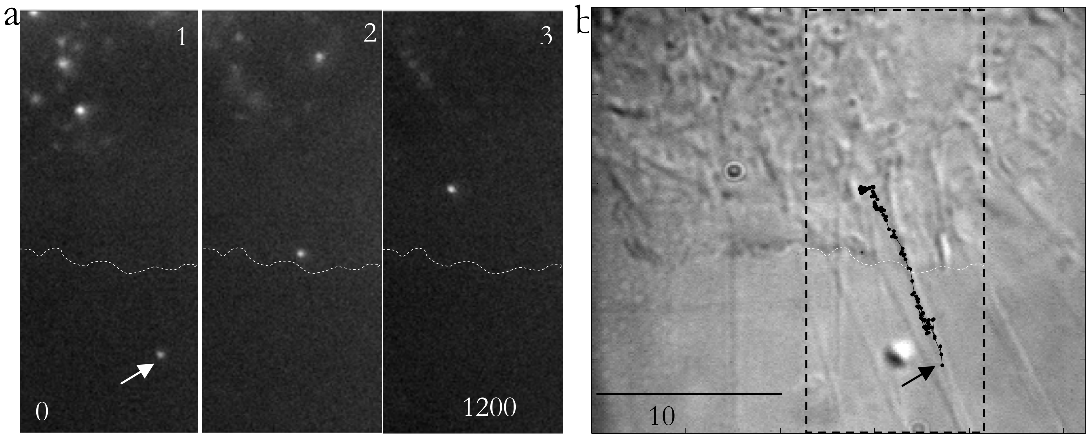


**Figure 2.** *The retrograde motion of 100-nm particles using single-molecule fluorescence techniques.*

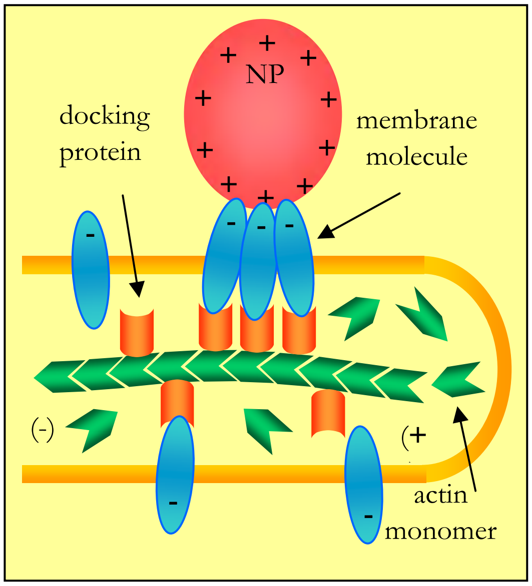


*Figure 3.* *Researchers found that the actin treadmilling powers the retrograde motion of the particles.*

By studying both negatively and positively charged particles, we found that only the positively charged particles can undergo a retrograde motion. This observation indicates that the motion is dependent on electrostatic interactions between negatively charged molecules in the plasma membrane and the positively charged surface of the particles. We also observed positively charged particles undergoing a retrograde motion in ATP depleted cells, which indicates that the motion is not powered by myosin or other ATP-dependent motor proteins. However, we found that the motion is strongly dependent on the integrity of the actin filaments within the microvilli. Actin filaments at the leading edge of many cells undergo a continuous cycle of assembly at their distal barbed end and disassembly at their proximal end. This treadmilling underlies a process termed actin retrograde flow. By transfecting the cells with fluorescent actin, which allowed us to follow the motion of actin clusters, and by applying drugs that inhibit the flow, we found that the actin treadmilling powers the retrograde motion of the particles, as illustrated in Figure 3.

The retrograde pathway brings a new mechanism by which positive surface charge supports particle recruitment, and potential subsequent toxicity, by polarized epithelial cells bearing microvilli.

Details of this research were recently published in *ACS Nano*. Movies of the imaging series can be accessed at http://pubs.acs.org/cgi-bin/article.cgi/ancac3/2007/1/i05/html/nn700149r.html. The article has been highlighted by colleagues in a special Perspective article at http://pubs.acs.org/cgi-bin/article.cgi/ancac3/2007/1/i05/html/nn700407v.html and in a podcast at http://pubs.acs.org/journals/ancac3/podcasts/index.html (episode 5).

**Citation**

Orr G, DJ Panther, JL Phillips, BJ Tarasevich, A Dohnalkova, D Hu, JG Teeguarden, and JG Pounds. 2007. “Submicrometer and Nanoscale Inorganic Particles Exploit the Actin Machinery to be Propelled along Microvilli-like Structures into Alveolar Cells.” *ACS Nano* 1(5):463-475.

# Zinc is Focus of Integrated Studies to Understand Metalloprotein Structure and Function

***AS Lipton,[(a)] RW Heck[(a)], M Valiev[(b)], WA de Jong[(b)], and PD Ellis[(a)]***

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

*Many critical biological functions, including DNA repair, depend on proteins with reactive metal centers. Understanding the structure of these proteins at the molecular level gives researchers insight into how those proteins carry out their very important jobs.*

Refining molecular theory using experimental data furthers researchers' understanding about the metal environment in structural and reactive sites of proteins, gaining strides in EMSL's focus to predict biological functions from molecular and chemical data.

Predictive models for metalloproteins are gaining accuracy because of integrated research using supercomputing and nuclear magnetic resonance spectrometry capabilities housed at DOE's EMSL. In a series of studies to relate metal-center protein environments to structure and function, a research team from EMSL and Pacific Northwest National Laboratory is using EMSL's NWChem computational chemistry software and NMR spectroscopy to derive a molecular theory that describes the electronic environment of the metal-amino acid motif, zinc coordinated to four cysteines. This motif was once thought to only play a structural role, but is now known to play a reactive role as well, for example, facilitating DNA repair.

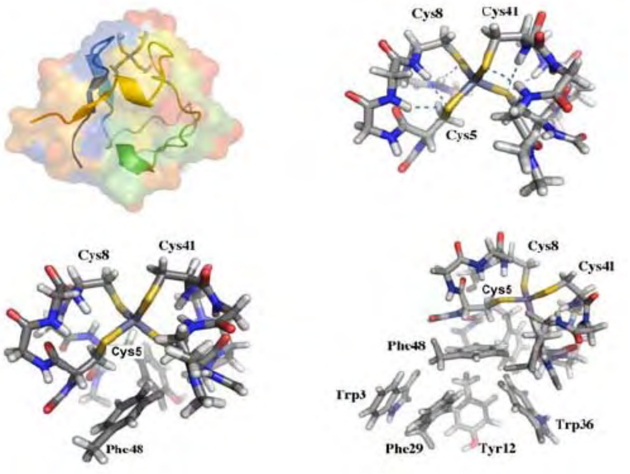


**Figure 1.** *Structure of the zinc- and cysteine-containing region of* Pyrococcus furiosis *rubredoxin determined with different computational chemistry models.*

In previous experiments, the research team used model proteins containing the zinc-cysteine motif to find a level of theory adequate to predict NMR results (Lipton and Ellis 2007). In the new phase of their studies described here, the team refined their model using a real-world example: zinc-substituted rubredoxin derived from the thermophile, *Pyrococcus furiosis* (Figure 1). Rubredoxins play a role in electron transfer – an important regulatory mechanism in biological systems. In zinc-substituted rubredoxin, the iron center of rubredoxin's active site is substituted with zinc, serving as a system of study for a zinc-cysteine site with only a structural role. To predict NMR data in this real-world scenario, computational theory requires a combination of quantum mechanics and molecular mechanics. In comparison to the level of computational theory required to describe the model proteins in previous studies, anisotropic shielding must be more heavily account for – in other words, NMR spectra peak characteristics measured at the zinc site are more dependent on the electron densities and the point of view of the observer for rubredoxin. In future studies, similar sites with reactive roles will be compared. This research was reported in the *Journal of the American Chemical Society* (Lipton et al. 2008).

**Citations**

Lipton AS, and PD Ellis. 2007. "Modeling the Metal Center of $Cys_4$ Zinc Proteins." *Journal of the American Chemical Society* 129(29):9192-9200.

Lipton AS, RW Heck, M Valiev, WA de Jong, and PD Ellis. 2008. "A QM/MM Approach to Interpreting $^{67}Zn$ Solid-state NMR Data in Zinc Proteins." *Journal of the American Chemical Society* 130(19):6224-6230.

## Energetics and Dynamics of Electron Transfer and Proton Transfer in Dissociation of Metal$^{III}$(salen)-Peptide Complexes in the Gas Phase

***J Laskin,[(a)] Z Yang,[(a)] and IK Chu[(b)]***
*(a) Pacific Northwest National Laboratory, Richland, Washington*
*(b) University of Hong Kong, Hong Kong, China*

*Peptides and proteins control nearly all of the chemical reactions in biological systems. This work studies the fundamental energetics and dynamics of model peptides in order to deepen the understanding of these biologically important molecules.*

Electron transfer and proton transfer are the most fundamental processes in chemistry and biology. Electron transfer is particularly important in enzyme catalysis, photosynthesis, and respiration. Gas-phase decomposition of ternary complexes of transition metal ions with organic and peptide ligands provides a unique opportunity to explore the competition between these processes using relatively simple model systems. It can also be used for the formation of different types of odd-electron peptide ions for analytical applications focused on identification of peptides and proteins using mass spectrometry.

Here we present the first detailed study of the energetics and dynamics of dissociation of positively charged metal$^{III}$(salen)-peptide complexes in the gas phase using time and collision-energy-resolved surface-induced dissociation (SID) experiments combined with RRKM modeling. Several fragmentation pathways are commonly observed during collision-induced dissociation of the positively charged metal-salen complexes. These include proton transfer to the peptide molecule or to the ligand, reduction of the metal center followed by electron transfer from the peptide molecule and formation of the radical cation, dissociation of the complex into the [metal$^{III}$(salen)]$^+$ ion and neutral peptide molecule (D), and dissociative electron transfer resulting in formation of fragment ions of the corresponding peptide radical cation. We examine factors that affect the competition between proton-transfer and electron-transfer processes in gas-phase fragmentation of these model systems.

Figure 1 shows a mass-selected [Co$^{III}$(salen)RVYIHPF]$^+$ precursor ion and its SID fragment distributions obtained at three collision energies. The four primary dissociation pathways are observed. Losses of $CO_2$ and COOH• are characteristic dissociation pathways of peptide radical cations that have been previously observed for dissociation of both doubly-charged and singly-charged ternary complexes of transition metals with peptides. Formation of these ions requires electron transfer from the peptide to the metal core of the complex. In addition, electron transfer results in formation of the peptide radical cation, $M^{+}$•, while the [M + H]+ ion is formed by proton transfer from the organic ligand to the peptide.

Time-resolved survival curves (SCs) were obtained by plotting the relative abundance of the intact precursor ion as a function of collision energy at different reaction delays. The SCs obtained at reaction delays of 1 ms and 1 s are shown for cobalt-salen complexes with three different peptides are displayed in Figure 2. The relative position of the SCs reflects the relative stability of different complexes toward fragmentation. The experimental SCs for $[Co^{III}(salen)DRVYIHPF]^{+}$ are slightly shifted toward higher collision energies for both 1 ms and 1 s reaction delays, while SCs obtained for cobalt-salen complexes of RVYIHPF and RVYIHDF show an almost perfect overlap. It should be noted that this trend follows the trend in the number of vibrational degrees of freedom (DOF) of the complexes (540 for DRVYIHPF, 501 for RVYIHPF, and 498 for RVYIHDF). The DOF effect can be eliminated by plotting the relative abundance of the precursor ion as a function of collision energy scaled by the number of DOF of the precursor ion. Perfect overlap between the SCs plotted versus the scaled collision energy clearly demonstrates that the observed shift in the position of the SCs shown results only from the DOF effect and suggests that both the energetics and dynamics of dissociation of all three cobalt-salen-peptide complexes are very similar.

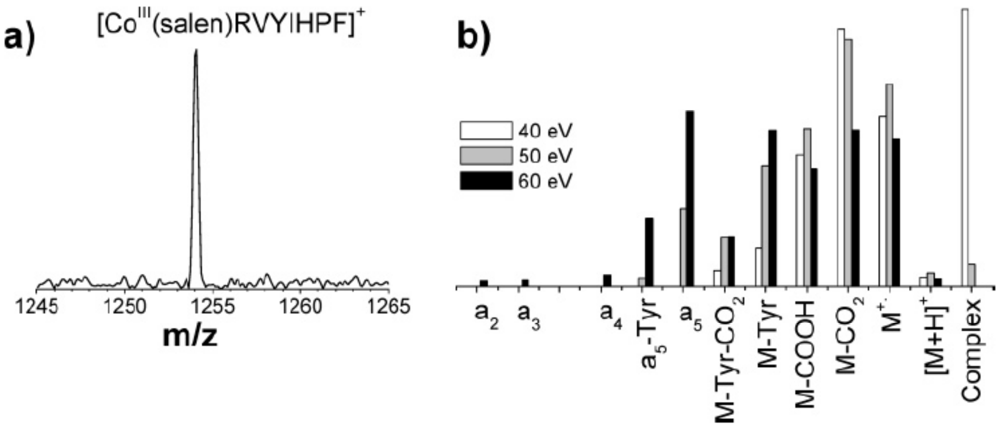


***Figure 1.*** *(a) Mass selected* $Co^{III}$*(salen)RVYIHPF precursor ion and (b) fragment distribution for SID of* $Co^{III}$*(salen)RVYIHPF complex on the HSAM surface at three collision energies.*

This work represents the first detailed study of the factors that affect gas-phase fragmentation of ternary complexes of angiotensin analogues with trivalent metal-salen systems. Time- and collision-energy-resolved SID provide interesting insight on the competition between proton transfer, electron transfer, and loss of the neutral peptide ligand in these model systems. We found that both the fragmentation behavior and the stability of

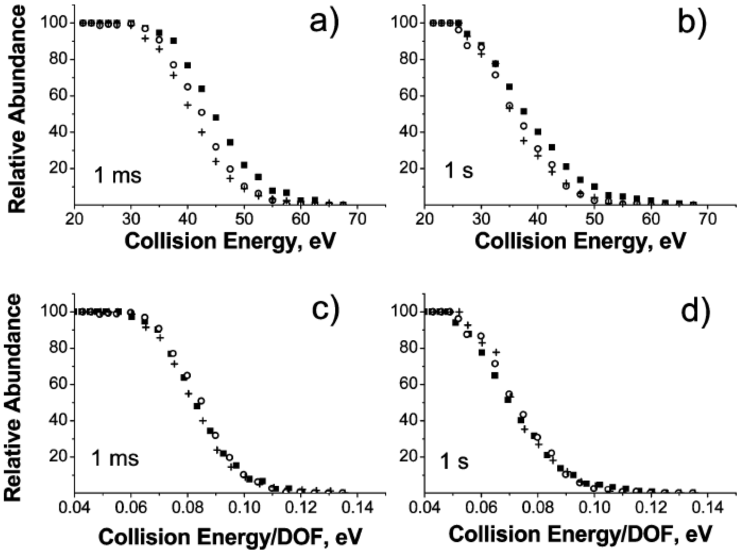


***Figure 2.*** *SCs (Panels a and b) and SCs plotted as a function of collision energy scaled by the number of the vibrational degrees of freedom of the precursor ion (Panels c and d) for Co$^{III}$(salen)DRVYIHPF (square), Co$^{III}$(salen)RVYIHPF (O), and Co$^{III}$(salen)RVYIHDF (+), 1 ms (left panels) and 1 s (right panels).*

the complexes are similar for different peptide ligands examined in this study. In contrast, the observed fragmentation pathways, the mode of binding, and the energetics and dynamics of dissociation of these systems strongly depend on the electronic properties of the metal center. Interestingly, a very different kinetics of formation of the M$^{+\bullet}$ fragment ion from the cobalt-salen and iron-salen complexes was observed experimentally. We concluded that the electron-transfer process in the dissociation of the [Fe$^{III}$(salen)RVYIHPF]$^+$ ion requires substantial rearrangement of the complex. Details of this exciting research were recently published in the *Journal of the American Chemical Society*.

**Citation:**

Laskin J, Z Yang, and IK Chu. 2008. "Energetics and Dynamics of Electron Transfer and Proton Transfer in Dissociation of Metal$^{III}$(salen)-Peptide Complexes in the Gas Phase." *Journal of the American Chemical Society* 130(10): 3218-3230.

# NMR Bioreactor Development for Live In-Situ Microbial Functional Analysis

***PD Majors[a], JS McLean [b], and JCM Scholten [c]***
*(a) Pacific Northwest National Laboratory, Richland, Washington*
*(b) The J. Craig Venter Institute, La Jolla, California*
*(c) Merck Co., Inc., West Point, Pennsylvania*

*An NMR bioreactor developed by EMSL users yields accurate metabolite profiles, metabolic pathways, and reaction rates without altering or depleting the sample. This research is one example of EMSL's move from static to dynamic studies in native environments.*

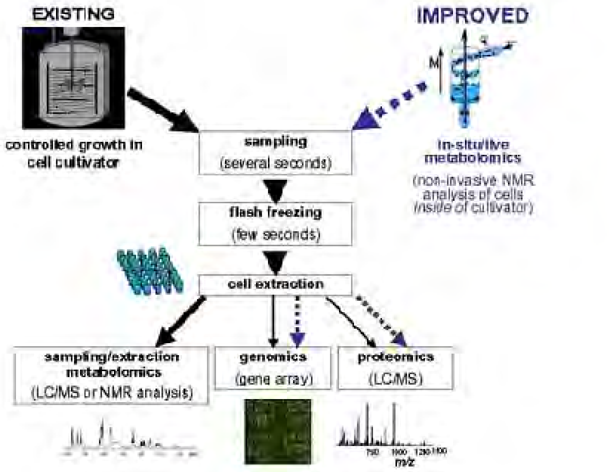


**Figure 1.** *The conventional technology (left) compared to the improved technology (right).*

Feeding microbes waste and having them convert it into valuable chemicals may sound far fetched, but scientists are closer, thanks to a new technology developed at EMSL. A first-of-its-kind MRI bioreactor (Figure 1) provides accurate metabolic information for live cells maintained in a controlled growth environment. Similar to clinical MRI, this *improved* technology uses noninvasive (nuclear) magnetic resonance imaging and spectroscopy (MRI/MRS) methods to monitor microbial metabolite concentrations *in the reactor* without removal or processing. This new technology provides a major advantage because metabolite levels can change significantly due to handling. Further, this technology allows for frequent, repeating measurements without diminishing the sample. Finally, it is compatible with high-throughput genomic and proteomic analyses.

The MRI/MRS bioreactor was used to study metabolites produced by *Eubacterium aggregans*, an anaerobic bacterium of interest for bio-fuel production. The study showed that in addition to known metabolic byproducts -- *E. aggregans* produces significant concentrations of lactate, a metabolite not previously reported. This suggests that the activities of its metabolic networks are different from what were predicted based on older experimental techniques. This research was featured on the cover of *Journal of Magnetic Resonance.*

## Citation

Majors PD, JS McLean, and JC Scholten. 2008. "NMR Bioreactor Development for Live In-Situ Microbial Functional Analysis." *Journal of Magnetic Resonance* 192(1):159-166.

# The Structure of the GAF A Domain from Phosphodiesterase 6C Reveals Determinants of cGMP-Binding, a Conserved Binding Surface, and a Large cGMP-Dependent Conformational Change

***SE Martinez[a], CC Heikaus[a], RE Klevit[a], and JA Beavo[a]***
*(a) University of Washington, Seattle, Washington*

*Determining the first structure of the photoreceptor phosphodiesterase bound to its ligand, cyclic guanosine monophosphate, is an important step for understanding ocular function. Studies such as this one support EMSL's goal to measure dynamic interactions in native environments and to predict biological functions from molecular and chemical data.*

The eyes house the elegant machinery that responds to photons and triggers the neural impulses that allow us to visualize our environment. Researchers from the University of Washington have used EMSL's nuclear magnetic resonance spectrometers and sophisticated probe technologies to gain new knowledge about the complex visual system at the molecular level. The team is the first to determine a high-resolution structure of the regulatory domain of the photoreceptor phosphodiesterase (PDE6) bound to its ligand, cyclic guanosine monophosphate (cGMP) (Figure 1). Studies such as this one are the first steps toward a fundamental understanding of the how the visual system works and how to fix it when it goes awry.

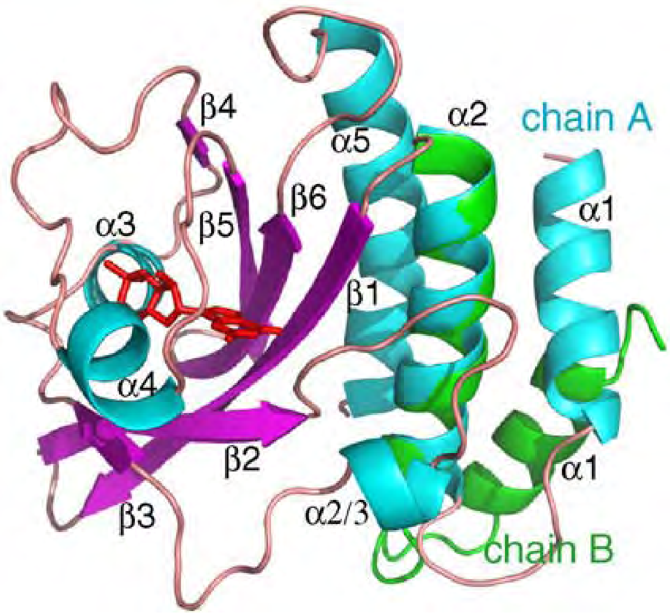


***Figure 1.** Structure of PDE6 GAF A bound to cGMP (red).*

The interaction between PDE6 and cGMP affects how *quickly* the eye can see. When it is activated by light, the regulatory region of PDE6, referred to as GAF A, activates PDE6. PDE6 in turn degrades cGMP, ultimately allowing the brain to receive information from the retina. Previous attempts to learn more about the ligand-free PDE6 GAF A domain via crystallization and diffraction studies were unsuccessful because crystals of the ligand-free protein are not easily prepared. So, the team turned to EMSL's NMR spectrometer and probe capabilities to investigate the conformational change of recombinant PDE6 while binding cGMP in real time and confirmed, at the atomic level, that GAF A is indeed the PDE6 binding site of cGMP.

This research was featured on the cover of *The Journal of Biological Chemistry*.

**Citation**

Martinez SE, CC Heikaus, RE Klevit, and JA Beavo. 2008. "The Structure of the GAF A Domain from Phosphodiesterase 6C Reveals Determinants of cGMP-Binding, a Conserved Binding Surface, and a Large cGMP-Dependent Conformational Change" *The Journal of Biological Chemistry* doi 10.1074/jbc.M802891200.

## Proteomic Characterization of the *Rhodobacter sphaeroides* 2.4.1 Photosynthetic Membrane: Identification of New Proteins

**X Zeng,[(a)] JH Roh,[(a)] SJ Callister,[(b)] CL Tavano,[(c)] TJ Donohue,[(c)] MS Lipton,[(b)] and S Kaplan[(a)]**
*(a) University of Texas Health Science Center, Houston, Texas*
*(b) Pacific Northwest National Laboratory, Richland, Washington*
*(c) University of Wisconsin-Madison, Madison, Wisconsin*

*The bacterium* Rhodobacter sphaeroides *2.4.1 is known for its diverse metabolic activities, including the ability to produce copious amounts of hydrogen, which could prove to be a source of renewable bioproduced energy. Many of these activities are linked to* R. sphaeroides' *photosynthetic apparatus that has served as a model for photosynthesis. Collaborative proteomic research being conducted at EMSL is increasing our understanding of this important link.*

This study builds upon previous proteomic research conducted at EMSL on *Rhodobacter sphaeroides* 2.4.1 (Callister et al. 2006a, 2006b) and details the discovery of new proteins associated with the intracytoplasmic membrane (ICM) (Figure 1), a specialized membrane dedicated to the photosynthetic processes used by *R. sphaeroides*. Subcellular fractionation combined with multichromatographic methods was coupled with Fourier transform ion cyclotron resonance mass spectrometry to test the hypothesis that a significant number of proteins associated with the ICM have not been previously been identified. The identification of these proteins could impact the understanding of how solar energy is used to the benefit of this organism.

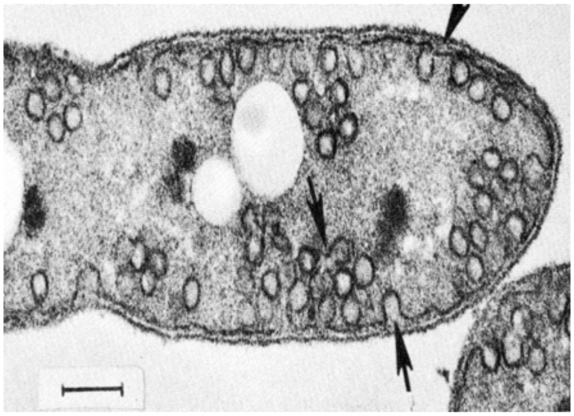


**Figure 1.** *The Intracytoplasmic Membrane (arrows) within* Rhodobacter sphaeroides 2.4.1 *houses proteins important for obtaining energy through photosynthesis. Using EMSL's proteomic capabilities, new proteins were discovered unique to the membrane.*

To evaluate this hypothesis, EMSL's proteomic capabilities were applied to probe the ICM for potentially important structural and metabolic proteins. ICM vesicles were purified from

*R. sphaeroides* cell cultures as well as surrounding sub-cellular fractions, such as the outer membrane, periplasm, and cytoplasmic membrane. Proteins extracted from the ICM and the other fractions were analyzed using a peptide-centric high-throughput liquid chromatography-mass spectrometry-based approach (Zimmer et al. 2006).

Purified ICM vesicles were shown to be enriched in several abundant, newly identified membrane proteins, including a protein of unknown function (AffyChip designation RSP1760) and a possible alkane hydroxylase (RSP1467). Deletion of the gene encoding for the RSP1760 protein resulted in the inability of *R. sphaeroides* to grow under conditions suitable for solar energy use, indicating the importance of this protein for *R. sphaeroides* to function as a photosynthesizing organism. Proteins necessary for other cellular functions, such as ATP synthesis, respiration, solute transport, protein translocation, and other physiological processes, were also identified to be in association with the ICM. This study is the first to provide a more global view of the protein composition of a photosynthetic membrane from any source. Results are provided in detail in the *Journal of Bacteriology* (Zeng et al. 2007).

**Citations**

Callister SJ, CD Nicora, X Zeng, JH Roh, MA Dominguez, CL Tavano, ME Monroe, S Kaplan, TJ Donahue, RD Smith, and MS Lipton. 2006a. "Comparison of Aerobic and Photosynthetic *Rhodobacter sphaeroides* 2.4.1 Proteomes." *Journal of Microbiological Methods* 67(3):424-436.

Callister SJ, MA Dominguez, CD Nicora, X Zeng, CL Tavano, S Kaplan, TJ Donahue, RD Smith, and MS Lipton. 2006b. "Application of the Accurate Mass and Time Tag Approach to the Proteome Analysis of Sub-cellular Fractions Obtained from *Rhodobacter sphaeroides* 2.4.1 Aerobic and Photosynthetic Cell Cultures." *Journal of Proteome Research* 5(8):1940-1947.

Zeng X, JH Roh, SJ Callister, CL Tavano, TJ Donahue, MS Lipton, and S Kaplan. 2007. "Proteomic Characterization of the *Rhodobacter sphaeroides* 2.4.1 Photosynthetic Membrane: Identification of New Proteins." *Journal of Bacteriology* 189(20):7464-7474.

Zimmer JSD, ME Monroe, WJ Qian, and RD Smith. 2006. "Advances in Proteomics Data Analysis and Display using an Accurate Mass and Time Tag Approach." *Mass Spectrometry Reviews* 25(3):450-482.

# Making Genomes Accessible: Dealing with the Avalanche of Biological Sequence Data

***VM Markowitz*[a]**

*(a) Lawrence Berkeley National Laboratory, Berkeley, California*

*The Integrated Microbial Genome system and its metagenome extensions are software tools that provide data management, analysis, and annotation capabilities for all publicly available microbial, viral, and eukaryal isolate genomes and metagenomes. Managing this collection of several thousand genomes and metagenomes requires performing trillions of pairwise sequence analysis calculations—a job which requires several years of computational time to complete. Using the Molecular Science Computing Facility supercomputer MPP2 and ScalaBLAST (specially designed high-throughput sequence analysis software from Pacific Northwest National Laboratory), these calculations have been periodically performed, leading directly to recent releases of Integrated Microbial Genome system and its metagenome extensions.*

The ability to recognize similarity in the DNA code that defines particular genes or proteins is a fundamental tool in molecular biology. When similar DNA or polypeptide sequences are observed, a biologist can infer homology, which is a family relationship based on inheritance from a common ancestor. Proteins that are homologous share a common three-dimensional structure that often allows their functions to be predicted. This type of evidence is powerful and underlies much of modern biology. The Integrated Microbial Genome (IMG) system and the metagenome extensions (IMG/M) (Markowitz 2007a, 2007b) are software resources built using homologous relationships between sequenced genomes for use by the biological research community. The IMG and IMG/M tool suites combine data management, analysis, and functional annotation capabilities based on pre-computed homologous relationships between publicly available genomes.

Two critical issues are exploding in importance in the large-scale sequence comparisons that must be performed to enable the IMG and IMG/M systems. First, building this basic map of sequence homology is becoming a significant obstacle because of the high throughput and cheap production of sequence data. The relatively few genes that have been *studied* experimentally must be projected against the majority that are *sequenced* but as yet uncharacterized. In 2007, there were about 400 microbial genomes alone that were completed, but this number is estimated to grow to 10,000 in just a few years. The scale of this dataset has outstripped various mechanisms that have been employed in the past to enhance the computational algorithm throughput of BLAST (Altschul et al. 1990), the basic method for comparing biosequences. The second issue relates to an exciting new type of analysis based on the comparison of genomes that has recently become possible precisely because there is so much data to work with. These genome comparison methods are essential for deciphering biological networks—a key step in enabling systems approach to biology. However, this more complex analysis typically consumes large numbers of sequence comparisons as raw material.

To deal with these large datasets, the researcher employed ScalaBLAST (Oehmen and Nieplocha 2006), which is a high-performance extension to the BLAST algorithm. ScalaBLAST was used to accelerate the throughput of BLAST sequence analysis using the

EMSL Molecular Science Computing Facility supercomputer MPP2 through a Computational Grand Challenge for several large-scale sequence analysis calculations. These calculations led directly to the 2.3 release of IMG and IMG/M and were directed at (1) integrating microbial genome and available metagenome data, and (2) applying this integrated data resource for specific scientific studies like advancing understanding of biological communities in the coastal margin between the Columbia River and Pacific Ocean.

**Citations**

Altschul SF, W Gish, W Miller, EW Myers, and DJ Lipman. 1990. "Basic Local Alignment Search Tool." *Journal of Molecular Biology* 215(3):403-410.

Markowitz VM, NN Ivanova, E Szeto, K Palaniappan, K Chu, D Dalevi, IA Chen, Y Grechkin, I Dubchak, I Anderson, A Lykidis, K Mavromatis, P Hugenholtz, and NC Kyrpides. 2007a. "IMG/M: A Data Management and Analysis System for Metagenomes." *Nucleic Acids Research*, Advance Access, in press.

Markowitz VM, E Szeto, K Palaniappan, Y Grechkin, K Chu, IA Chen, I Dubchak, I Anderson, A Lykidis, K Mavromatis, NN Ivanova, and NC Kyrpides. 2007b. "The Integrated Microbial Genomes (IMG) System in 2007: Data Content and Analysis Tool Extensions." *Nucleic Acids Research*, Advance Access, in press.

Oehmen C, and J Nieplocha. 2006. "ScalaBLAST: A Scalable Implementation of BLAST for High-Performance Data-Intensive Bioinformatics Analysis." *IEEE Transactions on Parallel and Distributed Systems* 17(8):740-749.

## Researchers Utilize Proteomics to Reveal a Core Proteome

***SJ Callister,[a] LA McCue,[a] JE Turse,[a] ME Monroe,[a] KJ Auberry,[b] RD Smith,[a] JN Adkins,[a] and MS Lipton[a]***

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

*Researchers leveraged proteomics technology at EMSL to reveal the existence of a core proteome among 17 diverse bacteria. While many researchers make genomic comparisons among different bacteria and often report a set of common genes or core genome (Koonin 2003), the expression of this core genome as a core proteome is not generally verified. The verification of these genes as proteins has important implications to defining a set of basal proteins important to bacterial life that could aid in the construction of synthetic life-like systems, or synthetic biology. Ultimately, this research demonstrated the ability to use proteomic data in a comparative manner outside of conventional norms.*

Enabled by a proteome database that encompassed ~967,000 experimentally determined unique peptides linked to specific protein information and publicly available genome sequences, the observation of proteins predicted from genomic comparisons among 17 environmental and pathogenic bacteria was investigated (Callister et al. 2008). Bacteria selected for this investigation included the metabolically diverse organisms *Rhodobacter sphaeroides*, *Shewanella oneidensis,* and *Synechocystis sp.* PCC6803, as well pathogens such as

*Yersina pestis* and *Salmonella typhimurium*. Facilitated by successful collaborations that have made samples available for proteomic analysis, this investigation represents the gathering and evaluation of proteomic measurements made over the past six years.

Genomic comparisons among the 17 bacteria predicted the existence of a core genome composed of 144 genes (Figure 1). Proteins from 74% of these genes were observed within the database, with each protein identified by two unique peptides. The large percentage of the core genome being observed surprised researchers because of the somewhat diverse make-up of the bacteria selected, and the different number and variety of conditions used to culture the organisms. This observation has led to the hypothesis that although the number of genes making up a core genome may expand or contract depending on the number and diversity of organisms included, the percent of these genes being expressed as proteins in nature will be high.

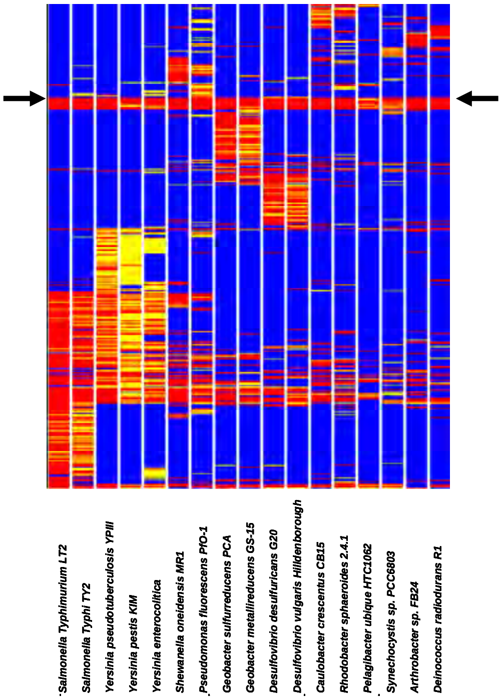


*Figure 1. The core proteome is revealed for 17 bacteria. Genomic comparisons identified genes common to two or more bacteria (orange) resulting in a core genome of 144 genes. Proteomic measurements were used to verify the existence of these genes as proteins (red) resulting in the identification of a core proteome (arrow).*

A functional analysis revealed that a majority of core proteome proteins (~55%) have functions related to protein synthesis, not surprising as the ability of a bacterial cell to make proteins for cell maintenance and growth is a vital function. However, what was surprising to researchers was the observation of proteins (~7%) having very little or no functional characterization; for example, the observation of the iojap-like protein. This gene was predicted in our study as homologous across all 17 bacteria and is also found outside the bacterial domain as well. The product of this gene is a small protein so the number of detectable peptides is also potentially small relative to some of the larger ribosomal proteins we observed. Yet, little is known about this protein's function in the bacterial cell (Galperin and Koonin 2004). The observation of these relatively uncharacterized proteins emphasizes the need for a better understanding of basal bacterial functions.

**Citations**

Callister SJ, LA McCue, JE Turse, ME Monroe, KJ Auberry, RD Smith, JN Adkins, and MS Lipton. 2008. "Comparative Bacterial Proteomics: Analysis of the Core Genome Concept." *PLoS ONE* 3(2):e1542.

Galperin MY, and EV Koonin. 2004. "'Conserved Hypothetical' Proteins: Prioritization of Targets for Experimental Study." *Nucleic Acids Research* 32(18):5452-5463.

Koonin EV. 2003. "Comparative Genomics, Minimal Gene-Sets and the Last Universal Common Ancestor." *Nature Reviews Microbiology* 1(2):127-136.

## Functional and Structural Characterization of DR_0079 from Deinococcus radiodurans, a Novel Nudix Hydrolase with a Preference for Cytosine (Deoxy)Ribonucleoside 5'-Di- and Triphosphates

***GW Buchko[(a)], O Litvinova[(b)], H Robinson[(c)], AF Yakunin[(b)], and MA Kennedy[(d)]***

*(a) Pacific Northwest National Laboratory, Richland, Washington*
*(b) University of Toronto, Toronto, Ontario, Canada*
*(c) Brookhaven National Laboratory, Upton, New York*
*(d) Miami University, Oxford, Ohio*

*A new function documented for a Nudix hyrdrolase of* D. radiodurans*, DR_0079, expands the range of possible Nudix substrates and provides an understanding of the molecular basis for* D. radiodurans *radiation-resistant properties, which may lead to novel bioremediation methods and to strategies that protect humans from the deleterious effects of ionizing radiation. Novel findings from real-time, molecular-level structure-function studies further EMSL's goals to predict biological functions from molecular and chemical data and to advance from static to dynamic studies in native environments.*

*Deinococcus radiodurans* can survive thousands of times more radiation exposure than a human. The biological mechanism for its radiation resistance may be related to an uncommonly large suite of housekeeping proteins called Nudix hydrolyases. A research team from Brookhaven National Laboratory, the University of Toronto, Miami University, and Pacific Northwest National Laboratory have used EMSL's state-of-the-art nuclear magnetic resonance spectroscopy capabilities to help determine the crystal structure for one of these *D. radiodurans* Nudix hydrolases, DR_0079, and uncovered its preference for a novel substrate (Figure 1).

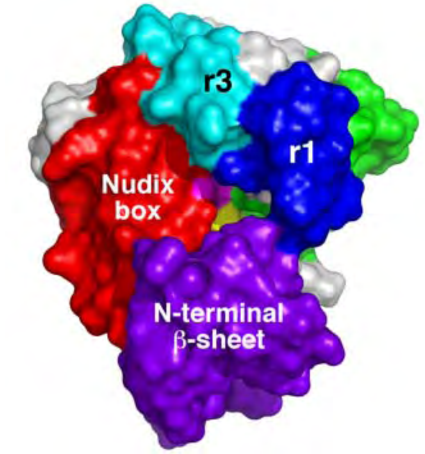


***Figure 1.** DR_0079 (205F) surface structure highlighting the Nudix box (red) and regions of the protein associated with substrate binding.*

Nudix hydrolyases are ubiquitous, existing in the genomes of organisms as diverse as viruses and humans. They are identified by a highly conserved, 23-residue consensus sequence, called the Nudix box, which forms part of the substrate-binding and catalytic site. The rest of a Nudix hydrolase's sequence determines the overall protein structure, which in turn influences substrate specificity. Substrates for Nudix hydrolases are typically nucleotide-based (related to the building blocks of DNA and RNA). The classic Nudix protein, MutT,

protects cells by converting dangerous promutagenic nucleoside triphosphates into safe nucleoside monophosphates – the former can be incorporated into DNA and lead to cancer, and the latter cannot. DR_0079 is unusual because it converts nucleoside *diphosphates* instead of nucleoside triphosphates into nucleoside monophosphates.

The team used X-ray diffraction data collected at the National Synchrotron Light Source to study the structure of DR_0079. To relate structure to function, the preferred substrate of the enzyme was verified and the molecular mechanism probed using $^{31}$P NMR spectroscopy at EMSL. This technique made it possible to study the protein's activity in real time and with molecular detail. This research was reported in *Biochemistry*.

**Citation**

Buchko GW, O Litvinova, H Robinson, AF Yakunin, and MA Kennedy. 2008. "Functional and Structural Characterization of DR_0079 from *Deinococcus radiodurans*, a Novel Nudix Hydrolase with a Preference for Cytosine (Deoxy)Ribonucleoside 5'-Di- and Triphosphates." *Biochemistry* 47:6571-82.

# Trapped-Ion Cell with Improved DC Potential Harmonicity for FT-ICR MS

***AV Tolmachev[(a)], EW Robinson[(a)], S Wu[(b)], H Kang[(b)], NM Lourette[(a)], L Pasa-Tolic[(c)], and RD Smith[(a)]***

*(a) Pacific Northwest National Laboratory, Richland, Washington*
*(b) Ajou University, Suwan, Korea*
*(c) EMSL, Richland, Washington*

*Using a more homogenous electric field in the FTICR, a mass spectrometric cell developed at EMSL is providign a two-fold increase in ion characterization. This work supports studies at EMSL to predict biological functions from molecular and chemical data.*

Whether studying proteins to identify methods for less invasive medical tests or discover hydrocarbons for new energy sources, scientists need instruments that provide reliable, accurate measurements. A new trapped-ion cell, designed and developed at EMSL, provides a two-fold improvement in mass accuracy. This increased accuracy allows scientists to more confidently analyze highly complex mixtures and distinguish between nearly identical molecules in samples.

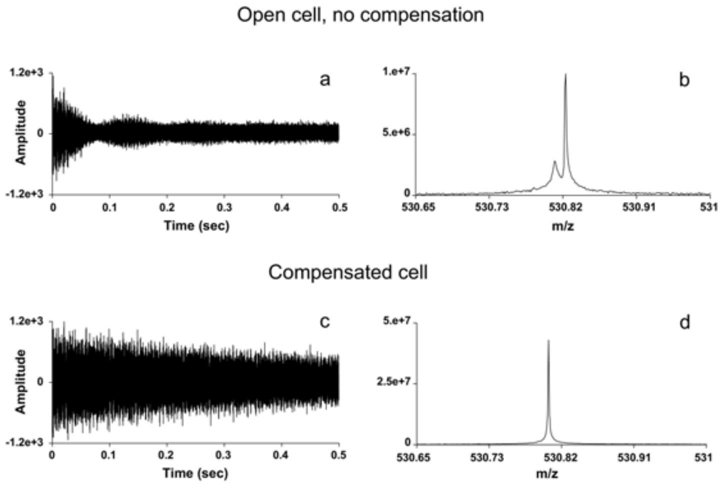


***Figure 1.** Peptide ions, coherently excited, induce a current on two detection plates using a conventional open cell (top left) and the new cell (bottom left). The more the ions are excited, the closer they get to the detection plates, which should increase the measured signal. However, in the open cell (top right), non-ideal electric fields distort the ion motion, resulting in peak splitting, reduced mass measurement accuracy, and reduced sensitivity. The more theoretically ideal electric fields in the new cell enable ions to be excited closer to the detection plates with significantly less distortion of the ion motion improving sensitivity (peak amplitude), dynamic range, and mass measurement accuracy. These improvements will result in more peptides (and therefore more proteins, especially less abundant proteins) being identified with greater confidence.*

The cell (Figure 1), designed by scientists from Pacific Northwest National Laboratory, Ajou University, and EMSL, is being used on several proteomics research projects in combination with EMSL's 12-Tesla Fourier transform ion cyclotron resonance mass spectrometer. The scientists began by studying the theories underlying FTICR and the accuracy obtained. Critical to the success of this mass spectrometry technique is the cell where the ions are trapped and excited. The new design generates an electrostatic trapping potential, responsible for holding the ions, that closely approaches the theoretical ideal. The new cell allows for higher signals and thus increased sensitivity and dynamic range.

Experimental characterization of the new cell confirmed that a more homogeneous electrostatic trapping field improves the FTICR's performance. This research was featured in *Journal of the American Society of Mass Spectrometry*.

**Citation**

Tolmachev AV, EW Robinson, S Wu, H Kang, NM Lourette, L Pasa-Tolić, and RD Smith. 2008. "Trapped-Ion Cell with Improved DC Potential Harmonicity for FT-ICR MS." *Journal of the American Society of Mass Spectrometry* 19(4):586-97.

# Backbone 1H, 13C, and 15N NMR Assignments for the Cyanothece 51142 Protein cce_0567: A Protein Associated with Nitrogen Fixation in the DUF683 Family

**GW Buchko[(a)] and HJ Sofia[(a)]**

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

*Understanding the structure of cce_0567 and other cyanobacteria proteins paves the way for further scientific inquiry, including biochemical experiments, into ubiquitous blue-green algae. This research is an example of EMSL's efforts to uncover biological functions from molecular and chemical data.*

As part of EMSL's Membrane Biology Grand Challenge, users have determined the crystal structure for the 78-residue protein cce_0567 from the cyanobacteria *Cyanothece sp. PCC 51142*. Studies suggest that the protein may play a role in nitrogen fixation and/or the circadian control of nitrogen fixation. Nitrogen fixation is the rate-limiting step in the growth of cyanobacteria. Understanding the proteins involved in nitrogen fixation could help unlock the mysteries of how to efficiently turn this ubiquitous algae into a carbon-neutral fuel.

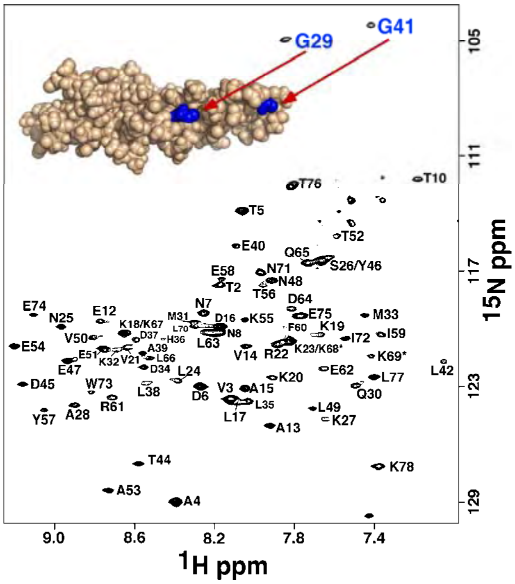


***Figure 1.*** *The assigned $^{1}H$-$^{15}N$ HSQC spectrum for cce_0567 with the crystal structure of the protein (3CSX) is shown near the top. Understanding the function of this protein may help scientists use blue-green algae for producing energy and sequestering carbon.*

Using EMSL's state-of-the-art resources, the nuclear magnetic resonance chemical shift assignments for cce_0567 were made using EMSL's 500-, 600-, 750-, and 800-MHz NMR spectrometers. The 1H -15N HSQC spectrum is a "fingerprint" for the protein's conformation. The assignment of the 1H -15N HSQC spectrum is an important step in probing the biological function of cce_0567 (Figure 1). Perturbations to these chemical shifts occur when other molecules are added to the solution. The perturbations are indicative of substrate binding. Following such chemical shifts allows researchers to identify protein-substrate interactions and then map them on to specific locations on the protein's surface using the structure determined by crystallographic methods. This research was published in *Biomolecular NMR Assignments*.

**Citation**

Buchko GW, and HJ Sofia. 2008. "Backbone 1H, 13C, and 15N NMR Assignments for the *Cyanothece 51142* Protein cce_0567: A Protein Associated with Nitrogen Fixation in the DUF683 Family." *Biomolecular NMR Assignments* 2(1):25-28.

## Researchers Integrate Computing with Experiments to Gain Insight in the Structure and Function of Enzymes and Peptides

*EMSL's experimental capabilities, combined with its computational modeling capabilities, provides fundamental insight into the structure and function of enzymes and proteins. This knowledge is essential for understanding the inner workings of biological systems.*

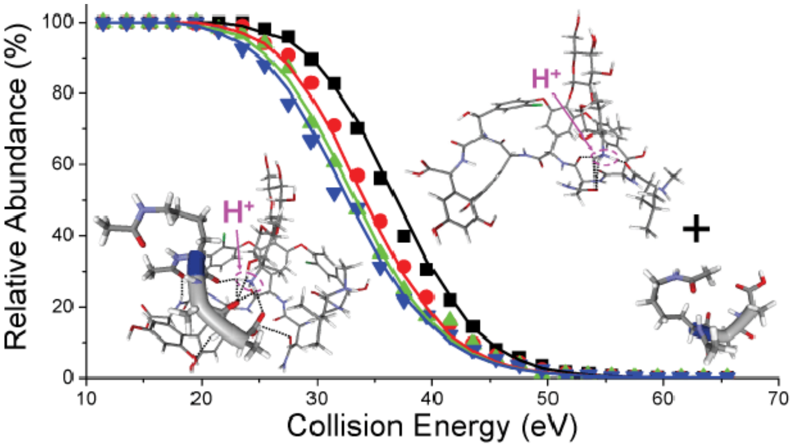


**Figure 1.***Fragmentation of the charged vancomycin-peptide complex (left) forms a protonated vancomycin and a neutral peptide molecule.*

One of EMSL's key characteristics is the integration of state-of-the-art experimental and computational capabilities. With all these capabilities under one roof, EMSL enables researchers to get access to a broad range of capabilities to solve some of the most important national challenges in energy, environmental sciences, and human health in a multidisciplinary fashion. Computational chemistry combined with large supercomputers has reached a level of accuracy such that simulations can help researchers interpret and understand complex experimental observations, or even guide experiments. Here two examples are highlighted where researchers have used experimental NMR or FT-CIR capabilities in conjunction with EMSL's NWChem software and supercomputer to gain knowledge about the inner working of biological systems.

Researchers from the University of Michigan and Pacific Northwest National Laboratory recently published an article in the top-ranking *Journal of the American Chemical Society*, describing how a combination of NMR experiments and insights from computational chemistry simulations lead to a detailed understanding of the structure and behavior of the Aquifex aeolicus LpxC enzyme in different environmental conditions. The scientists used EMSL's 500 and 800 MHz NMR and the NWChem software on EMSL's supercomputer to accomplish their research. Experiments have shown that the LpxC enzyme, which has a catalytic zinc ion in its center, reacts differently depending on pH. The main goal of this research was to identify at which pH the zinc-bound water of the enzyme, and also at which pH other parts of the enzyme get ionized. By calculating the NMR properties for various ionized enzyme structures, and comparing them with experimental data they were able to conclude that the water bound to the zinc ion in fact does not get ionized at all. Instead they found that two different side chains get deprotonated depending on the pH level.

Another article in the *Journal of the American Chemical Society*, researchers from Pacific Northwest National Laboratory demonstrated how the integration of theory and experiment can lead to a molecular-scale understanding of noncovalent interactions in biomolecular systems. In their research the scientists did surface-induced dissociation (SID) experiments with EMSL's 6 Tesla Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS) configured for studying ion-surface collisions, and theoretical calculations using EMSL's NWChem software and supercomputer. To probe the interaction of the vancomycin antibiotic with an analogue of a cell wall peptide ($N_a$,$N_e$-diacetyl-L-Lys-D-Ala-D-Ala), the researchers collided a protonated vancomycin-peptide complex with a surface to break it apart. This experiment allows them to obtain the binding energy between vancomycin and the peptide. Computational chemistry simulations were used to interpret the structure and composition of the complex. Comparison of binding energies obtained from different complexes modeled with theory and experiment provided the unique insight that the protonated complex really consists of a neutral peptide while the disaccharide group in vancomycin is protonated (Figure 1).

## Citations

Lipton AS, Heck RW, Hernick M, Fierke CA, and Ellis PD. 2008. "Residue Ionization in LpxC Directly Observed by $^{67}$Zn NMR Spectroscopy" *Journal of the American Chemical Society* 130: 12671-12679

Yang Z, Vorpagel ER, and Laskin J. 2008. "Experimental and Theoretical Studies of the Structures and Interactions of Vancomycin Antibiotics with Cell Wall Analogues" *Journal of the American Chemical Society* 130: 13013-13022

# Geochemistry/Biogeochemistry and Subsurface Science

One of the most challenging issues confronting DOE is the safe and cost-effective management of environmental pollutants and the remediation of hazardous waste sites. DOE is responsible for managing some 40 million cubic meters of contaminated soils and 1.7 trillion gallons of contaminated groundwater. At the Hanford Site in Richland, Washington, alone, DOE invests ~$2 billion a year in cleanup activities related to storing and processing radioactive waste in underground tanks and extensive remediation of soils and groundwater contaminated by past disposal practices and tank waste leaks. These issues are also national problems. For example, across the United States, thousands of Superfund sites exist with various levels and types of contamination such as organics, heavy metals, inorganics, and radionuclides. In the future, the subsurface migration of the byproducts of energy production, including nuclear waste and carbon dioxide, represents one of the most daunting challenges to DOE, and the safe and cost-effective disposal of these byproducts could be a limiting factor in deploying new energy technologies for the nation.

Molecular-level processes, such as aqueous complexation, adsorption to different mineral phases, or microbial reduction of redox active metals, often control the transport and fate of contaminants in the environment. These processes occur in chemically and physically heterogeneous subsurface environments. Understanding the structure, chemistry, and nanoscale geometric properties of mineral/water and microbe/mineral interfaces are critical to a mechanistic understanding of subsurface reactivity and contaminant transport. As a result, molecular-level studies of interfacial geochemistry and biogeochemical reactions have been an active area of research for more than a decade. Unraveling these phenomena at the molecular level and determining their impact on contaminant migration and transformation is a key objective of this science theme.

This science theme will focus EMSL's scientific resources on the following key topical areas:

- *Fundamental studies of interfacial molecular geochemistry and biogeochemistry*
- *Unraveling the chemistry of radionuclides in the subsurface*
- *Developing predictive transport models of chemical and microbial species in the subsurface.*

Research in the area of biogeochemistry and subsurface science is well established in EMSL. EMSL proposes to build on its strength in this area by advancing our capabilities to determine the chemical form of contaminants in complex subsurface materials, develop a fundamental understanding of dynamic interfacial processes and their impact on observed reactivity, and to improve our linkage of fundamental studies of molecular geochemistry/biogeochemistry to field scale transport processes.

Highlights of research performed in Fiscal Year 2008 under EMSL's Geochemistry/Biogeochemistry and Subsurface Science theme are shown below.

# Understanding Uranium Complex Formation through Combined Modeling and Gas-Phase Experiments

**WA de Jong,[a] GS Groenewold,[b] MJ Van Stipdonk[c], and L Visscher[d]**

(a) EMSL, Richland, Washington
(b) Idaho National Laboratory, Idaho Falls, Idaho
(c) Wichita State University, Wichita, Kansas
(d) Vrije Universiteit Amsterdam, Amsterdam, The Netherlands

*Using experimental analysis combined with EMSL's computational modeling capabilities, researchers obtained fundamental insight into the formation of uranium oxide complexes, knowledge that is essential for understanding the speciation of uranium in the subsurface and in Hanford waste tanks.*

The production of radioactive materials has resulted in large amounts of waste and releases of radioactive constituents at DOE sites and in the environment. Gaining a comprehensive description and full understanding of contaminant mobility represents a major challenge to DOE's cleanup mission, as the transport and transformation of contaminants in the subsurface and across key groundwater-surface water interfaces is not well understood. In the dynamic realm of solution-phase actinide coordination chemistry, the formation and stability of complexes is controlled by coordination, geometry, oxidation state, and cooperative effects between different ligands. Probing these aspects provides fundamental insight that is leading to an understanding of the effect of electronic structure and bonding preferences that could eventually be exploited to manipulate actinide behavior.

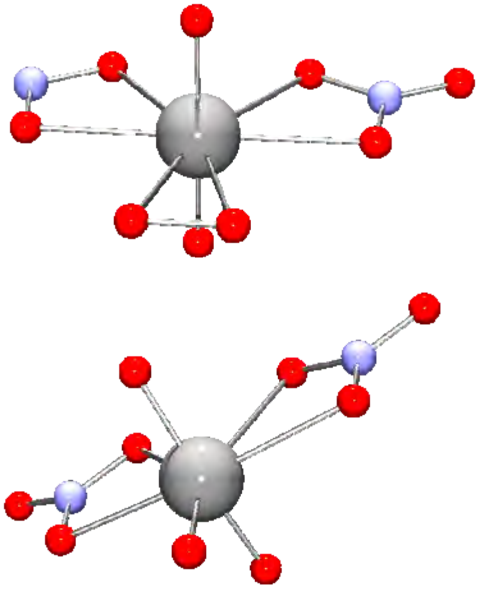


**Figure 1**. *Possible uranyl nitrate complexes formed after photofragmentation. Top: $[UO_2(NO_3)_2O]^-$, Bottom: $[UO_2NO_3NO_2O_2]^-$.*

Researchers from Idaho National Laboratory and Wichita State University have used infrared multiple photon dissociation experiments to probe the formation and reactivity of uranyl-ligand ($UO_2^{2+}$) complexes in the gas-phase, controlling the type of ligands, number of ligands, and oxidation state of the uranyl. Infrared spectra of the formed complexes and photo-fragmentation pathways were obtained from the experiments, but to obtain a complete understanding and interpretation of their observations, the researchers teamed up with computational chemists from EMSL and the Vrije Universiteit Amsterdam. Using EMSL's supercomputer and NWChem computational chemistry software, the researchers were able to obtain molecular structures, vibrational spectra, and reaction energetics that reproduced the experimental observations with reasonable accuracy, leading to a comprehensive interpretation of the results.

A comprehensive study of uranyl-nitrate complexes, readily present in Hanford Site waste tanks, was recently published in *Physical Chemistry Chemical Physics* (Groenwald et al. 2008a). The $[UO_2(NO_3)_3]^-$ was irradiated, but instead of losing a nitrate ligand, an $NO_2$ fragment dissociated from the complex. Infrared spectra did not provide the insight of the complex formed as either $[UO_2(NO_3)_2O]^-$ or, through a complex reaction mechanism, the superoxide $[UO_2NO_3NO_2O_2]^-$ could be formed (Figure 1). Comparing the results of computational modeling of different complex geometries and their associated infrared spectra with the experimental data revealed that the uranyl-nitrate complex dissociated to and from the $[UO_2(NO_3)_2O]^-$ complex.

An article published in the high-ranking *Journal of Physical Chemistry A* (Groenwald et al. 2008b) describes the formation of $[UO_2A(S)_n]^+$ complexes, where A was a hydroxide, methoxide, or acetate, while S (ranging from one to three ligands) was water, ammonia, acetone, or acetonitrile. Computational modeling showed that there is a clear correlation between the ligand dissociation energy and ability to donate electron density to the uranyl ion, and changes in the infrared asymmetric stretch of the uranyl. Generally, the computational results were found to be in good agreement with the experimental data. The only exception is the disagreement between theory and experiment for the free $UO_2OH^+$, which is still not fully explained. One possible cause could be anharmonicity, as the spectra are measured by pumping in energy and breaking the molecule. For this small a molecule, anharmonicity might become important, or excited states might be involved.

## Citations

Groenewold GS, J Oomens, WA de Jong, GL Gresham, ME McIlwain, and MJ Van Stipdonk. 2008a. "Vibrational Spectroscopy of Anionic Nitrate Complexes of $UO_2^{2+}$ and $Eu^{3+}$ Isolated in the Gas Phase." *Physical Chemistry Chemical Physics (PCCP)* 10(8):1192-1202.

Groenewold GS, AK Gianotto, ME McIlwain, MJ Van Stipdonk, M Kullman, DT Moore, N Polfer, J Oomens, I Invante, L Visscher, B Siboulet, and WA de Jong. 2008b. "Infrared Spectroscopy of Discrete Uranyl Anion Complexes" *Journal of Physical Chemistry A* 112(3):508-521.

# Carbon Tetrachloride Flow and Transport in the Subsurface of the 216-Z-9 Trench at the Hanford Site

***M Oostrom,[(a)] ML Rockhold,[(a)] PD Thorne,[(a)] MJ Truex,[(a)] GV Last,[(a)] and VJ Rohay[(a)]***

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

*Using a combined modeling and experimental approach, this study determined that the future threat of carbon tetrachloride contamination of Hanford groundwater comes from the interaction between groundwater and carbon tetrachloride vapor and not migration of residual carbon tetrachloride liquid. As a result, remediation strategies are being refined to target the carbon tetrachloride vapor threat.*

As a result of past practices, up to 580 m$^3$ carbon tetrachloride was discharged to waste sites at the 200 West Area of the U.S. Department of Energy's Hanford Site near Richland, Washington. Three-dimensional modeling was conducted to enhance the current conceptual model of $CCl_4$ distribution beneath the major disposal site (216-Z-9). The simulations, using the STOMP code, focused on migration of dense nonaqueous-phase liquid (DNAPL) consisting of $CCl_4$ and co-disposed organics under scenarios with differing sediment properties, sediment distribution, waste properties, and waste disposal history. Simulation results support a conceptual model for $CCl_4$ distribution where $CCl_4$ in the DNAPL phase migrated primarily in a vertical direction below the disposal site and where some $CCl_4$ DNAPL likely migrated across the water table into the regional aquifer. Results also show that the lower permeability Cold Creek unit retained more $CCl_4$ DNAPL within the vadose zone than other hydrologic units during the infiltration and redistribution process. Because of the relatively high vapor pressure of the $CCl_4$, the resulting vapor plumes are extensive and influenced by density-driven advection. Any continued migration of $CCl_4$ from the vadose zone to the groundwater is likely through interaction of vapor phase $CCl_4$ with the groundwater and not through continued DNAPL migration.

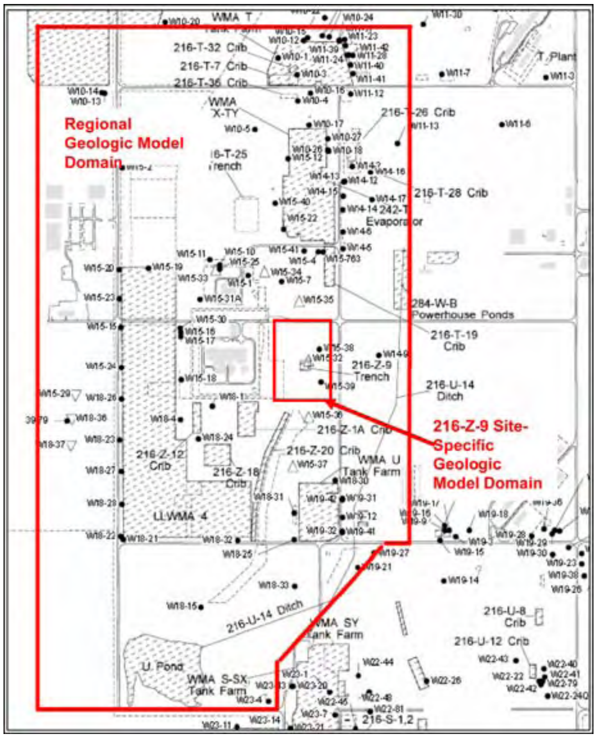


**Figure 1.** *Outline of regional and 216-Z-9 trench geologic model domains at the Hanford Site.*

Additional simulations assessed the impacts of soil vapor extraction (SVE) as a remediation method. These simulations showed rapid $CCl_4$ removal associated with the assumed local equilibrium of $CCl_4$ between the phases. Additional efforts are needed to enhance the understanding of rate-limited volatilization to improve simulation of the SVE process and to provide a basis for refining the design and operation of SVE systems.

Plutonium recovery operations within the 200 West Area resulted in organic and aqueous wastes that were disposed of at several cribs, tile fields, and French drains. The organic wastes consisted of $CCl_4$ mixed with lard oil, tributyl phosphate, and dibutyl butyl phosphonate. The main disposal areas were the 216-Z-9 trench, the 216-Z-1A tile field, and the 216-Z-18 crib. These three major disposal facilities received a total of about 13,400,000 liters of liquid waste containing 363,000 to 580,000 liters of $CCl_4$. The disposal site locations are shown in Figure 1, with the 216-Z-9 site situated in the middle of the site-specific model domain and the 216-Z-1A and 216-Z-18 sites located to the southwest of the site-specific domain. The Plutonium Finishing Plant is directly to the west of the 216-Z-9 disposal site. Assuming a maximum aqueous $CCl_4$ solubility of 800 $mg{\cdot}L^{-1}$ and an organic liquid density of 1.59 $g{\cdot}cm^{-3}$ (Schwille 1988), the 13,400,000 liters of liquid waste would be able to contain approximately 6700 liters of $CCl_4$ in dissolved form, indicating that the majority of the $CCl_4$ entered the subsurface as an organic liquid.

In recent years, two major remediation technologies have been applied to remove $CCl_4$ from the vadose zone and groundwater at the Hanford Site. Beginning in 1991, about 78,000 kg of $CCl_4$ was removed using an SVE system in the vadose zone (Fluor Hanford 2006). In addition, a pump-and-treat system for the unconfined aquifer removed 9700 kg of $CCl_4$ from the groundwater beginning in 1994 (DOE 2006).

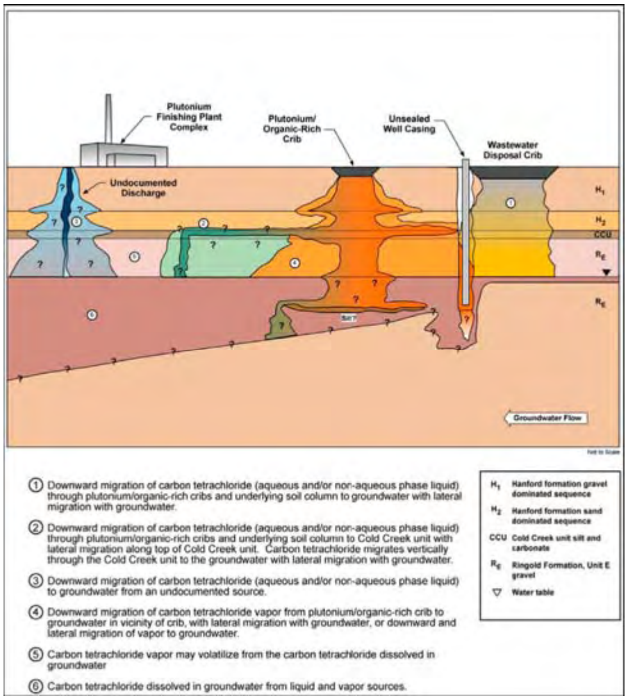


**Figure 2.** *Current conceptual model of subsurface carbon tetrachloride behavior* (after DOE 2004).

The main objective of the current study is to develop an updated conceptual model for $CCl_4$ behavior under the 216-Z-9 site, based on a series of multifluid flow simulations, and compare the updated conceptual model with the existing model described by DOE (2004), as shown in Figure 2. The numerical simulations focus on the 216-Z-9 site because of the three major DNAPL disposal sites, the 216-Z-9 has the smallest footprint and has received the most DNAPL waste. Because of these characteristics, it is expected that DNAPL disposed at the 216-Z-9 trench may have moved deeper into the subsurface compared to the other Hanford $CCl_4$ disposal sites. A series of three-dimensional multifluid flow simulations was conducted using the STOMP code (White and Oostrom 2006), including a base case simulation and 28 sensitivity analysis simulations, to examine the impact of parameter variation on the simulated migration of $CCl_4$ in the subsurface beneath the 216-Z-9 disposal area from 1954 to 2005. An additional objective was to investigate the impact of SVE, implemented at the site in 1993, on $CCl_4$ distributions and fluxes. This research was recently published in *Vadose Zone Journal* (Oostrom et al. 2007).

**Citations**

Fluor Hanford. 2006. Performance Evaluation Report for Soil Vapor Extraction Operations at the 200-PW-1 Carbon Tetrachloride Site, Fiscal Year 2005. WMP-30426, Fluor Hanford, Richland, Washington.

Oostrom M, ML Rockhold, PD Thorne, MJ Truex, GV Last, and VJ Rohay. 2007. "Carbon Tetrachloride Flow and Transport in the Subsurface of the 216-Z-9 Trench at the Hanford Site." *Vadose Zone Journal* 6(4):971-984.

Schwille F. 1988. *Dense Chlorinated Solvents.* Lewis Publishers, Chelsea, Michigan.

U.S. Department of Energy. 2004. *Plutonium/Organic-Rich Process Condensate/Process Waste Group Operable Unit RI/FS Work Plan, Includes: 200-PW-1, 200-PW-3, and 200-PW-6 Operable Units.* DOE/RL-2001-01, Rev. 0, reissue. DOE, Richland Operations Office, Richland, Washington.

U.S. Department of Energy. 2006. *Fiscal Year 2005 Annual Summary Report for 200-UP-1 and 200-ZP-1 Pump-and-Treat Operations.* DOE/RL-2005-91. DOE, Richland Operations Office, Richland, Washington.

White MD, and M Oostrom. 2006. *STOMP Subsurface Transport Over Multiple Phases, Version 4.0 Users Guide.* PNNL-15782. Pacific Northwest National Laboratory, Richland, Washington.

## Geochemical Controls on Contaminant Uranium in Vadose Hanford Formation Sediments at the 200 Area and 300 Area, Hanford Site, Washington

***JP McKinley,[a] JM Zachara,[a] J Wan,[b] DE McCready,[c] and SM Heald[d]***

*(a) Pacific Northwest National Laboratory, Richland, Washington*
*(b) Lawrence Berkeley National Laboratory, Berkeley, California*
*(c) Environmental Molecular Sciences Laboratory, Richland, Washington*
*(d) Argonne National Laboratory, Argonne, Illinois*

*Using combined experimental analysis and electron microscope imaging, this study determined that secondary mineral formation is the dominant control of uranium contamination of Hanford Site groundwater.*

Long-term historic spills of uranium at the Hanford Site's 300 Area fuel fabrication site (58,000 kg of disposed uranium over 32 years) and at the 200 East Area BX tank farm (7000 kg of spilled uranium in one event), both within the Hanford formation near Richland, Washington, were investigated by subsurface sampling and subsequent microscale investigations of excavated samples. The 200 Area sediments contained uranyl silicate mineralization (sodium boltwoodite) in restrictive microfractures in granitic clasts, in the vadose zone over a narrow range in depth. Well logging and column experiments indicated that tank wastes migrated deeper than observed in core samples. The 300 Area sediments included metatorbernite and uranium at low concentrations associated with detrital aluminosilicates, along with other mineral phases that could accommodate uranyl, such as uranophane and calcium carbonate. The association of contaminant uranyl with Hanford formation sediments provided a persistent source of uranium to groundwater. The results of both studies suggest that the formation of secondary solid uranyl-bearing phases influences the subsequent release of uranium to the environment and that our understanding of these processes and individual waste sites is incomplete.

The Hanford Site produced plutonium from 1943 until 1989 for weapons applications. The Site occupies about 1500 $km^2$ in an arid environment, bounded by a broad bend of the Columbia River to the east and by Rattlesnake Mountain to the west. Fuel fabrication occurred at the Site's southern extremity (300 Area); fuel was irradiated near the Columbia River to the north (100 Area); and the rods were processed in chemical facilities on the Site's central plateau (200 Area). Each of the manufacturing components had a characteristic waste stream or streams, and while some streams were disposed directly onto the ground surface, others were retained for long-term storage or isolation. Materials research and fabrication at the 300 Area generated wastes that were sluiced into process ponds (Figure 1, top), constructed and maintained to avoid contamination of the nearby Columbia River.

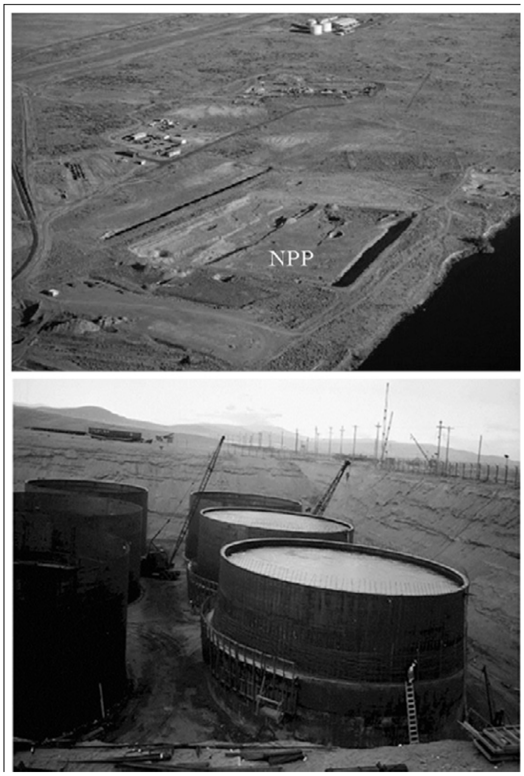


**Figure 1**. *Top: Aerial photograph of the 300 Area North Process Pond, in 2003, after excavation of the residual pond wastes. Samples described here were removed from the site after this photo was taken. Bottom: Photograph of the 200 East Area BX tank farm under construction, 1944.*

The ponds received constant and intermittent releases of a broad variety in composition and volume, including caustic alkaline and acidic fluids and slurries containing uranium, aluminum, and copper. After irradiation, the chemical processing steps in the 200 Area included dissolution of irradiated fuel rods and subsequent industrial-scale chemical manipulations to form distinct compositional streams that were managed to extract useful materials and to isolate wastes. The storage of chemical process intermediates and the disposal of unwanted wastes presented (and continues to present) a significant challenge. During the years of plutonium production, highly radioactive and hazardous wastes were disposed in underground tanks (Figure 1, bottom), which were initially of single-wall construction.

The unintended release of uranium and other wastes to the environment produced contaminated zones in the vadose sediments. This study focused on two distinct contaminant events: (1) a historic, episodic leak of alkaline uranium wastes to the thick and deep 200 East Area vadose zone, and (2) the long-term seepage of acidic or neutral uranium wastes to the thin and shallow 300 Area vadose zone. Both released uranium into the same surficial sedimentary deposit, and each represents the source or potential source of uranium to groundwater.

The mobility of uranium is a complex function of the chemical and physical properties and the geological and lithological variations in the subsurface. The present-day geochemical behavior of the wastes appears to be controlled by the composition and morphologic character of the secondary waste-bearing solid phases, which in turn result from the composition and reactivity of the original aqueous waste, which migrated through the vadose environment. The results of these investigations also illustrate the uncertainties and difficulties in understanding the geochemical factors controlling potential environmental hazards of long-resident contaminants in the vadose regime. More detail is provided in *Vadose Zone Journal* (McKinley et al. 2007).

**Citation**

McKinley JP, JM Zachara, J Wan, DE McCready, and SM Heald. 2007. "Geochemical Controls on Contaminant Uranium in Vadose Hanford Formation Sediments at the 200 Area and 300 Area, Hanford Site, Washington." *Vadose Zone Journal* 6(4):1004-1017.

## *In Vitro* Evolution of a Peptide with a Hematite Binding Motif That May Constitute a Natural Metal-Oxide Binding Archetype

***BH Lower[a], RD Lins[a], ZW Oestreicher[b], TP Straatsma[a], MF Hochella, Jr.[c], L Shi[a], and SK Lower[b]***

*(a) Pacific Northwest National Laboratory, Richland, Washington*
*(b) The Ohio State University, Columbus, Ohio*
*(c) Virginia Tech, Blacksburg, Virginia*

*This research answers a fundamental question in polypeptide binding and could aid researchers in everything from better understanding geochemical processes to designing and controlling material synthesis for biofuel cells. This work is part of EMSL's continued effort to link theory and simulations to experiments in real time.*

A diverse team of geologists, biologists, and computer scientists from the Pacific Northwest National Laboratory, The Ohio State University, and Virginia Tech is looking into how microorganisms bind to iron oxide. These interactions, common in the subsurface, are of importance to understanding the transport of environmental contaminants and subsequent remediation. Using computational and experimental resources at EMSL, the team found the protein fragment or polypeptide, just 9 amino acids long, that glues the larger protein to iron oxide.

To find this binding polypeptide, the team began with phage technology, using a virus to create more than 3 billion different polypeptides. They screened these molecules and found the polypeptide that would bind to hematite. Next, they performed molecular simulations using an AMBER96 force field with EMSL's NWChem. The simulations showed that the polypeptide takes on a shape that matches the mineral surface, allowing it to grip the surface

(Figure 1). Finally, the team searched the genomes of numerous bacteria to see if the polypeptide existed in microbes known for their interactions with metal oxides and found the sequence in *Thalassiosira pseudomona* and *Shewanella oneidensis*. This research was featured in *Environmental Science and Technology*.

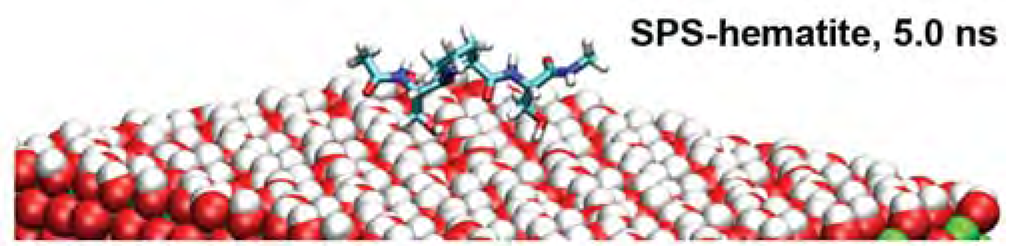


***Figure 1.*** *Snapshot of the SPS-hematite simulation at 5.0 ns. The peptide adopts a conformation that allows its two serine residues to form hydrogen bonds with hematite and template the iron oxide surface.*

**Citation**

Lower BH, RD Lins, ZW Oestreicher, TP Straatsma, MF Hochella, Jr., L Shi, and SK Lower. 2008. "*In Vitro* Evolution of a Peptide with a Hematite Binding Motif That May Constitute a Natural Metal-Oxide Binding Archetype." *Environmental Science and Technology* 42(10):3821-3827.

# Science of Interfacial Phenomena

Interfaces control many chemical and physical properties of natural and engineered materials critical to environmental- and energy related research and technologies important to the mission of DOE and to society in general. The importance of interfaces has been highlighted in DOE workshops covering topics including geosciences, solid-state lighting, solar energy, and advanced nuclear energy systems.

Tailored or designed surfaces and interfaces are important as model systems for detailed study of processes that occur on natural heterogeneous materials in the environment and for developing materials with new properties for energy production, catalysis, or other uses.

The behaviors of complex heterogeneous materials in the environment may never be fully understood without model systems that allow specific aspects of that complexity to be examined in detail. Likewise, material systems with interfaces optimized with specific properties are essential for the technologies needed for a secure environment and a stable energy future. Understanding these often complex interfaces requires methods to characterize naturally complex materials and minerals found in the environment and to understand increasingly complex materials designed and synthesized to have a desired functionality.

The Science of Interfacial Phenomena science theme is focused on understanding and gaining control of structure-function relationships at the atomic level to allow the design of new energy technologies and to understand the behaviors of natural systems. Topics of major emphasis in this science theme include the following:

- *Catalytic structure-function relationships to allow precise control of catalytic activity and selectivity.*
- *Gaining critical knowledge of photocatalysis and photochemistry.*
- *Design material systems with specialized charge and mass transport properties.*

The science and technological issues that need to be addressed to achieve these goals complement and to some degree naturally intersect those of the other science themes. The ability to characterize surfaces and small particles also provides a natural pathway for addressing issues of atmospheric aerosol chemistry. Developing technologies that rely on improved understanding and control of molecular-level structural, dynamic, and transport properties of interfaces include the following:

- New generations of selective catalysts
- Thin-film solar cells
- Solid-state lighting
- Hydrogen production and storage
- Solid-oxide fuel cells
- Chemical sensors and radiation detectors
- Materials for next-generation nuclear reactors.

Research capabilities and expertise in EMSL enable the design of a variety of material systems with specialized atomic, electronic, ionic transport properties and interfacial properties. Because of their environmental importance EMSL has become a premier laboratory for the study of oxide materials and mineral surfaces. These materials have an increasing importance in fuel cells, catalysis, sensors, advanced electronics, photovoltaics and solid state lighting and continue as one area of special expertise.

Highlights of research performed in Fiscal Year 2008 under EMSL's Science of Interfacial Phenomena science theme are shown below.

## Transient Mobility of Oxygen Adatoms upon $O_2$ Dissociation on Reduced $TiO_2$ (110)

***Y Du,[(a)] Z Dohnálek[(b)] and IV Lyubinetsky[(a)]***
*(a) EMSL, Richland, Washington*
*(b) Pacific Northwest National Laboratory, Richland, Washington*

*The interaction of molecular oxygen with $TiO_2$–based materials can affect many chemical and photochemical processes. In particular, it plays an important role in a wide range of applications such as photocatalysis, degradation of organic pollutants, and water splitting for hydrogen production.*

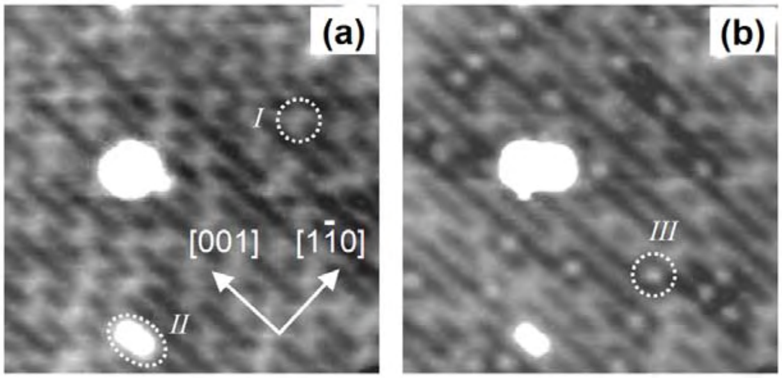
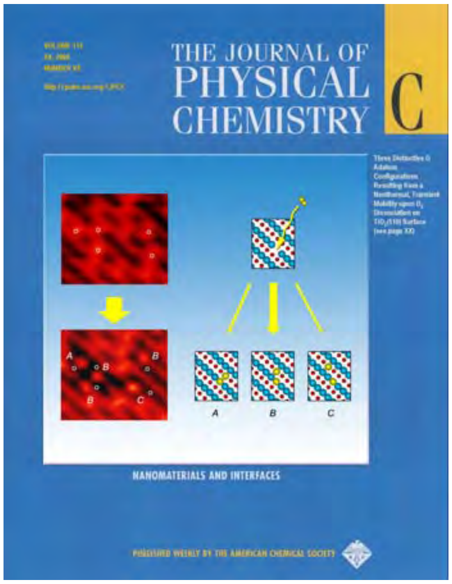


***Figure 1.*** *Scanning tunneling microscopy images of the same (11 × 10) $nm^2$ area of the $TiO_2$ (110) surface (a) before and (b) after adsorption of 0.03 ML of $O_2$ at 300 K. One of the oxygen vacancies, double hydroxyl group, and oxygen adatom are labeled with I, II, and III, respectively.*

Oxygen vacancy-mediated dissociation of $O_2$ molecules on $TiO_2$ (110) is shown to be energetically favorable by a number of theoretical investigations. On the basis of temperature-programmed desorption observations, researchers have suggested that for each $O_2$ molecule dissociated at the vacancy, one oxygen atom fills a vacancy while the other oxygen atom resides on the surface as an adatom, bound to the nearest-neighbor five-fold coordinated titanium site in the adjacent titanium row. The oxygen adatoms are found to significantly perturb the surface chemistry of adsorbed water, ammonia, and methanol, and may as well alter the surface chemistry of other adsorbate species on the $TiO_2$(110).

Recently, using *in-situ* scanning tunneling microscopy, the researchers studied at the atomic level the initial stages of $O_2$ dissociation at room temperature by tracking the same surface area before and after oxygen exposure. The results confirm that $O_2$ molecules dissociate only at the bridging oxygen vacancies, resulting in the healing of a vacancy by one oxygen atom, $O_v$, and the deposition of the other oxygen as an adatom, $O_a$, on a neighboring five-fold coordinated titanium site as shown in Figure 1.

After dissociation, the majority (~81 %) of O adatoms were found to separate from the original vacancy positions by up to two lattice constants along [001] direction. The majority of the adatoms (~74 %) were one lattice constant apart along [001] direction from the original vacancy positions shown as configuration *B* in Figure 2 (published as cover of *The Journal of Physical Chemistry C*). Other $O_a$ atoms were separated by two lattice constants (~7 %, configuration *C* in Figure 2) or bonded at the nearest-neighbor titanium sites (~19 %, configuration *A* in Figure 2). Studies showed that a limited nonthermal, transient mobility resulting from energy release during $O_2$ dissociation, rather than thermal diffusion was accounted for the observed distribution. Effect of the hyperthermal transient mobility of the oxygen adatoms may lead to an enhanced reactivity, which could be of a general relevance for the chemical and photochemical processes involving oxygen interaction with $TiO_2$-based systems.


THE JOURNAL OF PHYSICAL CHEMISTRY C

NANOMATERIALS AND INTERFACES

PUBLISHED WEEKLY BY THE AMERICAN CHEMICAL SOCIETY

***Figure 2.*** *Three different oxygen adatom configurations resulting from a nonthermal transient mobility upon* $O_2$ *dissociation on* $TiO_2$ *(110) surface.*

**Citation**

Du Y, Z Dohnálek, and I Lyubinetsky. 2007. "Transient Mobility of Oxygen Adatoms upon $O_2$ Dissociation on Reduced $TiO_2$ (110)." *Journal of Physical Chemistry C* 112(7):2649-2653.

## Probing Reaction Pathways Using *in situ* $^1$H NMR Spectroscopy

***L Shaw,[a] JZ Hu,[b] JH Kwak,[b] and Z Yang[b]***

*(a) University of Connecticut, Storrs, Connecticut*
*(b) Pacific Northwest National Laboratory, Richland, Washington*

*Real-time observation of the reaction mechanisms for the generation of* $H_2$ *will help researchers identify potential hydrogen storage materials.*

In collaboration with Professor Leon Shaw's group from the University of Connecticut, Drs. Jian Zhi Hu, Ja Hun Kwak and Zhenguo Yang from PNNL used *in situ* variable temperature

$^1H$ nuclear magnetic resonance (NMR) spectroscopy to observe the products produced during controlled conditions. The results gave direct evidence of the two-step reaction pathway for evolution of $H_2$ in the dehydrogenation reaction:

$$LiNH_2+LiH=Li_2NH+H_2. \quad (1)$$

This Li-N-H system, first reported by Chen et al., has been extensively investigated as potential hydrogen storage material. It was shown that decomposition is rapid in the order of 25 milliseconds, and several studies have hinted that a two-step mechanism existed (see Equations 2 and 3).

$$LiNH_2 = 1/2Li_2NH + 1/2NH_3 \quad (2)$$

$$1/2NH_3 + 1/2LiH = 1/2\ LiNH_2 + 1/2H_2. \quad (3)$$

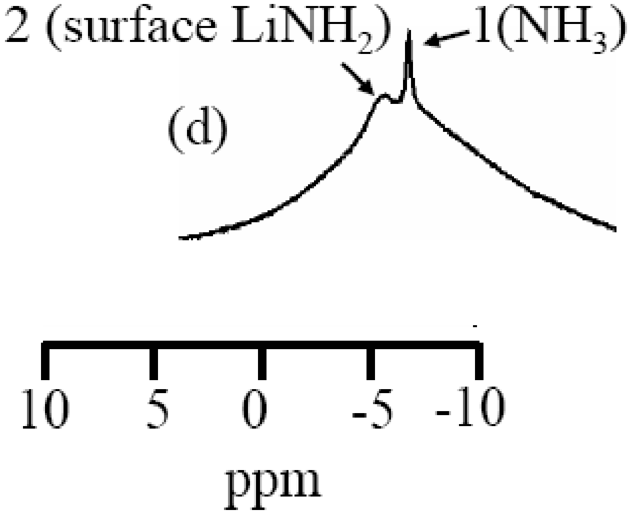


**Figure 1.** *$^1H$ spectrum of $LiNH_2$ power acquired at 30°C, which highlights the molecules attributed to surface $LiNH_2$ and the $NH_3$ released at 30°C.*

Results from this *in-situ* experiment at EMSL resulted in definitive direct evidence for the two-step mechanism. The results were published online (http://dx.doi.org/10.1016/j.jpowsour.2008.03.034), and a paper is in press for publication in *Journal of Power Sources* (an ISI Top-5 journal in energy and fuels).

During the variable temperature *in-situ* NMR experiment performed on a powder sample of $LiNH_2$ that was prepared using high-energy ball milling, three separate peaks were identified in the subsequent $^1H$ spectra (Figure 1). These peaks verified the existence of bulk $LiNH_2$, surface $LiNH_2$, and gaseous $NH_3$. All assignments were assisted by understanding the connection of line width to molecular motion. In particular, fast motion on the NMR time scale leads to narrow lines and rigid slow motion to wide lines.

Changing the temperature conditions shows that $NH_3$ was released slowly at 30°C and the speed of ammonia release significantly increased at temperatures above 75°C.

The variable temperature *in-situ* NMR experiments (Figure 2) on a powder sample consisting of a mixture of $LiNH_2$ + LiH that was mechanically activated via high-energy ball milling reveals the observation of $NH_3$, indicating that reaction (3) is not very fast until temperatures above 150°C are reached and that the minimum temperature required activating (2) is lower than the temperature required to activate (3). The appearance of $NH_3$ peak in Figure 2(d) and the disappearance of the $NH_3$ peak in Figure 2(f) clearly confirm the two elementary reaction steps [i.e., $NH_3$ is generated first by $LiNH_2$ (see Equation (2) and then $NH_3$ reacts with LiH to release $H_2$ (Equation (3)].

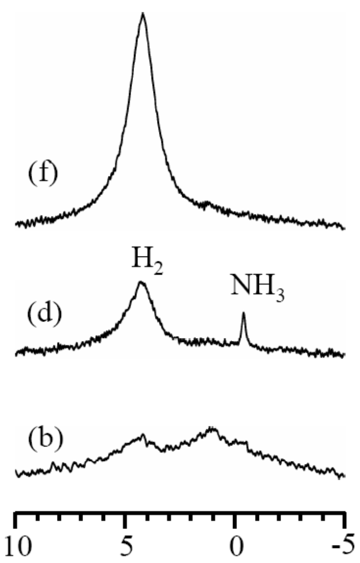


***Figure 2.*** *Representative in situ $^1H$ NMR spectra of the $LiNH_2$ + LiH samples. Spectrum (f) was acquired when the temperature was ramped from 150°C to 180°C (no $NH_3$ peak observed). Trace Spectrum (d) was acquired when the temperature was ramped from approximately 40°C to 150°C. Both the $NH_3$ product from Equation 2 and the $H_2$ product from Equation 3 are observed. Spectrum (b) was acquired at room temperature.*

The *in-situ* techniques developed here serve to illustrate the potential application of a relatively simple approach that will enable the real-time observation of mechanistic data and performance evaluation in future hydrogen storage material studies.

**Citation**

Chen P, Z Xiong, J Luo, J Lin, and KL Tan. 2002. "Interaction of Hydrogen with Metal Nitrides and Imides." *Nature* 420(6913): 302-304.

# A Multinuclear MAS NMR Investigation of the Environmentally Relevant Material Magnesium Aluminum Layered Double Hydroxides

***JL Palumbo,*** $^{(a)}$ ***PJ Sideris,*** $^{(a)}$ ***and CP Grey*** $^{(a)}$

*(a) State University of New York at Stony Brook, Stony Brook, New York*

*Magnesium aluminum layered double hydroxides serve as an anion exchange material that can remove toxic anions such as selenates, arsenates and halides from wastewater. The detailed structure of these materials has been unknown, and this work uses nuclear magnetic resonance to determine their structure, which is important to understanding how to develop new materials that are more selective or effective in the role of treating wastewater. The results of this research were reported in* Science.

The anion-exchange ability of layered double hydroxides (LDHs) has been exploited to create materials for use in catalysis, drug delivery, and environmental remediation. The specific cation arrangements in the hydroxide layers of hydrotalcite-like LDHs, of general formula $Mg^{2+}_{1-x}Al^{3+}_{x}OH_2(Anion^{n-}_{x/n})\cdot yH_2O$, have, however, remained elusive, and their elucidation could enhance the functional optimization of these materials. The presence of a trivalent metal in the metal hydroxide $[M_{1-x}M'_{x}(OH)_2]$ sheet induces an overall positive charge, which is compensated by the incorporation of the anion, along with structural water, in the interlayer spaces (Figure 1). One naturally occurring example of this class of materials is the mineral hydrotalcite, $Mg_6Al_2(OH)_{16}CO_3\cdot 4H_2O$, which contains carbonate ions in between the layers. The use of several nuclear magnetic resonance (NMR) techniques, including high-speed magic angle spinning (MAS), Multiple Quantum MAS (MQMAS), and high-field NMR spectra on a 900-MHz spectrometer have combined to give a clear picture of the atomic organization of hydrotalcite which has not been possible using other techniques.

We looked at several compositions of hydrotalcite with varying amounts of aluminum, up to 33% aluminum on a molar ratio, so we could compare how the spectra changed with composition. Particular attention was paid to the naturally occurring form with a 2:1 ratio of magnesium to aluminum. If the metal sites were randomly distributed, there would be a distribution of the hydroxide sites with 1, 2, 3 or 4 nearest aluminum neighbors. The NMR data indicate that the hydroxide sites are next to either 0 or 1 aluminum neighbors, indicating that the aluminum sites are not randomly distributed, but are part of an ordered structure where no more than one aluminum site is near a hydroxide group.

21.1-Tesla (900-MHz) NMR data from magnesium samples of brucite ($Mg(OMg)_6$), 19% aluminum, 25% aluminum, and 33% Al LDH's show that both the brucite and the 33% aluminum LDH have strong axial symmetry, but the quadrupolar properties of the magnesium are different between the two samples. This indicates that the magnesium spectrum is sensitive to the addition of aluminum to the structure, even though the overall structure is not changed by the substitution of aluminum for magnesium. The magnesium NMR data from the intermediate concentrations of aluminum show the presence of both the brucite signal and the 33% aluminum LDH signal, demonstrating a nice transition between forms as more aluminum is added to the material.

Figure 1 demonstrates the structure of the 33% aluminum LDH with the bound anions between the sheets of the LDH in A. B shows a random distribution of hydroxide groups, which is not what was found, and C shows the ordered arrangement which was discovered.

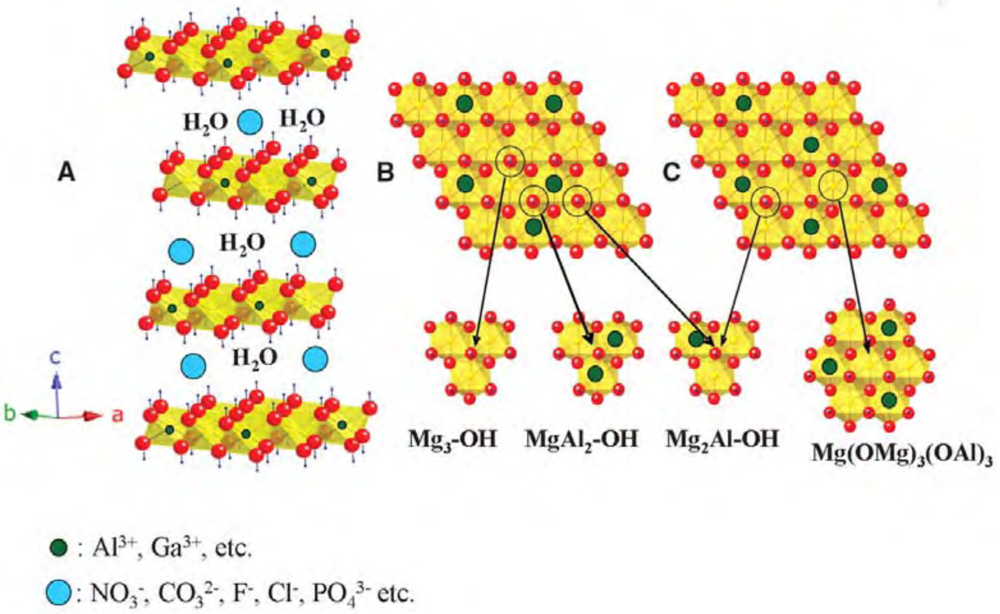


***Figure 1. (A)*** *A polyhedral representation of the LDH structure showing the metal hydroxide octahedra stacked along the crystallographic c axis. Water and anions are present in the interlayer region. Each hydroxyl group (dark blue) is oriented toward the interlayer region and may be hydrogen-bonded to the interlayer anions and water. The metal hydroxide sheets of an LDH with a Mg:Al ratio of 2:1 are shown with (**B**) random and (**C**) ordered cation distributions. Three major classes of hydroxyl groups are present in (B) ($Mg_3$-OH, $Mg_2Al$-OH, and $MgAl_2$-OH), whereas only one hydroxyl environment ($Mg_2Al$-OH) and one Mg local environment [$Mg(OMg)_3(OAl)_3$] are present in (C).*

## Citation

Sideris PJ, UG Nielsen, Z Gan, and CP Grey. 2008. "Mg/Al Ordering in Layered Double Hydroxides Revealed by Multinuclear NMR Spectroscopy." *Science* 321(5885):113-117.

# Nuclear-spin Relaxation of $^{207}$Pb in Ferroelectric Powders

**LS Bouchard[(a)], AO Sushdov[(b)], D Dudker[(a,b)], JJ Ford[(c)], and AS Lipton[(d)]**

(a) Lawrence Berkeley National Laboratory, Berkeley, California
(b) University of California at Berkeley, Berkeley, California
(c) EMSL, Richland, Washington
(d) Pacific Northwest National Laboratory, Richland, Washington

*Certain fundamental properties of matter are still not fully understood at the atomic and subatomic level. One such property is the Schiff moment, which can be present in high atomic weight nuclei and violates the parity (P) and time reversal (T) symmetries of standard quantum mechanics. Materials with high ferroelectric moments, such as lead titanates, present the opportunity to measure a Schiff moment on a macroscopic scale. However, there is a lot of preliminary work needed before the Schiff moment can be observed and measured, including the work presented here.*

Motivated by a recent proposal by Sushkov and co-workers to search for a P,T-violating Schiff moment of the $^{207}$Pb nucleus in a ferroelectric solid, we have carried out a high-field nuclear magnetic resonance study of the longitudinal ($T_1$) and transverse ($T_2$) spin relaxation of the lead nuclei from room temperature down to 10 K for powder samples of lead titanate (PT), lead zirconium titanate (PZT), and a PT monocrystal.

Ferroelectric solids have unique properties, including the presence of a macroscopic electric field, which makes them useful in many electronic devices, including sensors. Their properties also make them suitable to observe and measure the presence of a P,T violating Schiff moment. The temperature range to be studied was from room temperature down to 10K. As the samples cooled, the $T_1$ should increase and the rate of increase would be a reflection of the relaxation processes involved. With the need to vary the temperature over such a wide range, there is very little equipment capable of making this measurement. However, a custom probe designed and built at EMSL has the required range for this set of experiments, and we were able to make use of this unique resource for these experiments.

$T_2$ data collected over the entire temperature range indicated a constant $T_2$ of about 1 ms for all samples. This is consistent with a dipole-dipole relaxation mechanism for $T_2$ relaxation. As seen in Figure 1, the $T_1$ data is considerably more interesting. At temperatures above 50 Kelvin, all of the samples had a linear relationship between temperature and relaxation rate ($1/T_1 \propto T^2$). This is characteristic of a two-phonon Raman process, a relaxation mechanism investigated and explained in terms of modulation in the spin-rotation interaction. There is a temperature (the Debye temperature) below which this process would become dependent $T^7$. The $T_1$ data below 50K does not follow this behavior, but instead follows a more complicated behavior. This behavior is consistent with paramagnetic impurities being present in the samples and, at low temperatures, this becomes the dominant source of $T_1$ relaxation. Over the course of the temperature range, the $T_1$ increases from 10 seconds at room temperature to one hour at 10K. These research results were reported in *Physical Review A*.

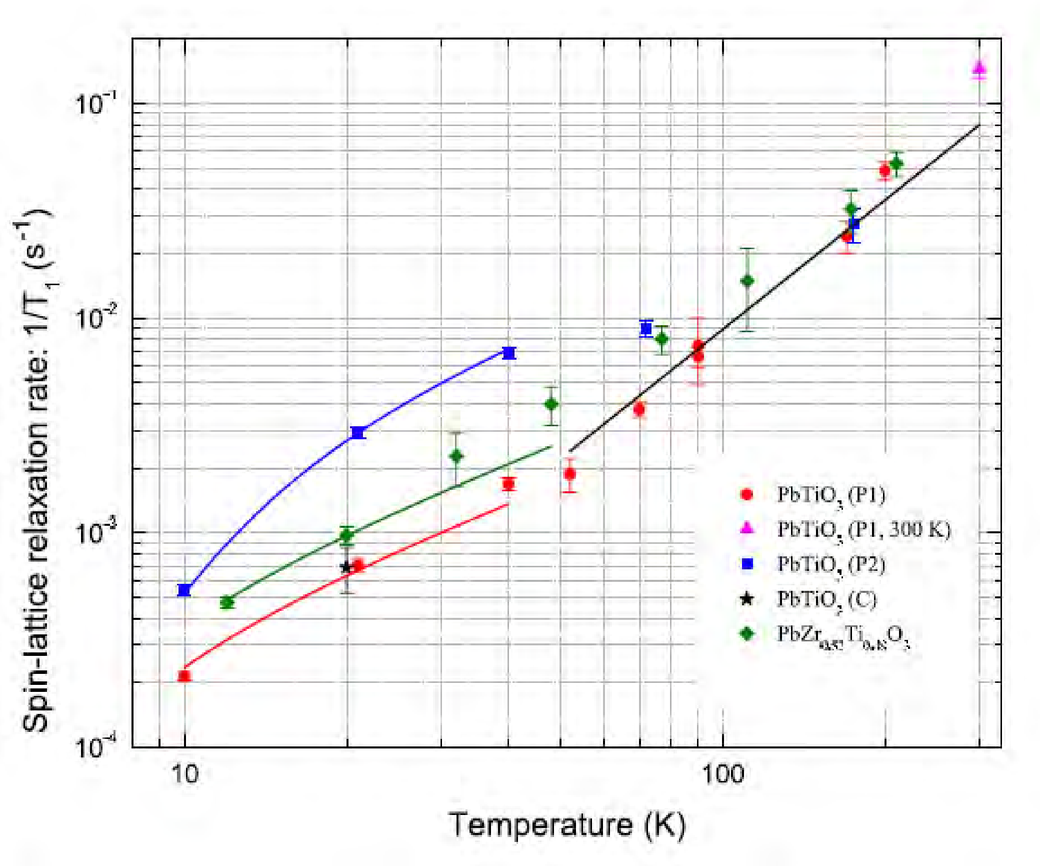


***Figure 1.*** *Graph of Relaxation rate ($1/T_1$) versus temperature.*

The presence of paramagnetic impurities may actually be useful in the effort to observe Schiff moments in using $^{207}$Pb nuclear magnetic resonance. To observe the Schiff moment, the temperature needs to be dropped to less than 1K. This would be done by cooling the sample to 1K and then demagnetize the sample to cool it further. A one-hour $T_1$ is convenient because that is not too long to achieve full polarization of the sample, but long enough to make the necessary measurements to observe the Schiff moment. Two main questions remain to be answered in future investigations: what is the spin-lattice relaxation time in low magnetic fields and low spin temperatures, and does the presence of paramagnetic impurities introduce serious systematics into the Schiff-moment-induced magnetization search? We are currently developing experiments to address both of these questions.

## Citation

Bouchard LS, AO Sushkov, D Budker, JJ Ford, and AS Lipton. 2008. "Nuclear-Spin Relaxation of $^{207}$Pb in Ferroelectric Powders." *Physical Review A* 77(2):022102 (6 pages).

# One Step Closer to Hydrogen-Powered Cars

**J Knudson,[a] AU Nilekar,[b] RT Vang,[a] J Schadt,[a] EL Kunkes,[b]**
**JA Dumesic,[b] M Mavrikakis,[b] and F Besenbacher[a]**
(a) University of Aarhus, Aarhus, Denmark
(b) University of Wisconsin-Madison, Madison, Wisconsin

*One key technological advance needed to enable efficient widespread use of hydrogen fuel cells for transportation involves the water-gas-shift (WGS) reaction ($CO + H_2O \rightarrow CO_2 + H_2$). This reaction is a crucial step in hydrogen production from fossil fuels. There is need for a better catalyst for small-scale applications before this process can be used in hydrogen fuel cell powered vehicles. Part of an EMSL Computational Grand Challenge project on Computational Design of Catalysts focuses on uncovering the details of the WGS reaction and is led by Manos Mavrikakis at the University of Wisconsin, Madison. High-performance computing using EMSL's supercomputer is an essential tool in probing the molecular details of how a proposed copper-platinum alloy might facilitate the WGS reaction.*

Scientists using EMSL's supercomputer have been running calculations on a new alloy as a potential catalyst for the water-gas-shift (WGS) reaction—a key capability in making hydrogen fuel cell vehicles a commercially viable reality. The crux of the study is to characterize the energy requirements for creating the alloy and understanding the details of how it interacts with the WGS reaction. Using computational chemistry software, the energetics of constructing a copper/platinum (Cu/Pt) near-surface alloy and its catalytic properties were analyzed. The alloy was found to have copper preferentially incorporated in the subsurface layer of platinum, meaning that creating the alloy is energetically favorable. Large-scale calculations and experimental x-ray photoelectron spectroscopy results both show copper is most stable in the first subsurface layer of a platinum lattice. A comparison between the experimental and theoretically simulated scanning tunneling microscope images (Figure 1) reveals that post-annealing, the subsurface layer of the alloy is copper-rich. Additionally, experiments on carbon-monoxide (CO) desorption from the catalyst suggest that with increasing copper coverage, the CO-desorption temperature would decrease.

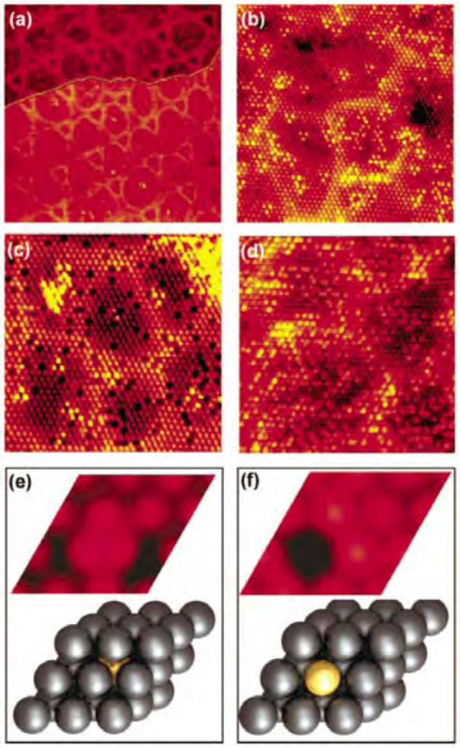


**Figure 1.** *Experimental and density functional theory-simulated scanning tunneling microscopy images. A comparison between the experimental and theoretically simulated scanning tunneling microscopy images reveals that post-annealing, the subsurface layer of the alloy is copper-rich.*

Using computational methods, this relationship between CO desorption and temperature holds only if copper is in the subsurface layer. These calculations and observations confirm the ideal configuration of copper and platinum can be assembled in an energy-efficient process because incorporation of copper into the platinum lattice is chemically favored at typical annealing temperatures.

The study also found that the Cu/Pt alloy has promising properties as a potential catalyst for the WGS reaction. CO binds more weakly to a special form of the alloy—Cu/Pt nitrosyl sulfuric acid (NSA)—than to a pure platinum surface. In addition, a common spectator/poison of WGS catalysts, formate (HCOO), binds more weakly than copper, suggesting that formate will not fatally interfere with this catalyst. Perhaps most importantly, Cu/Pt NSA activates water—the rate limiting step for WGS—as efficiently as copper, and yet binds the water dissociation products much more weakly than copper. This facilitates subsequent steps in the hydrogen production pathway. All these properties make the Cu/Pt NSA alloy a promising candidate for WGS catalysis, one that could be more active with a higher stability against poisoning by dominant reactive intermediates. The results were published in the *Journal of the American Chemical Society* (Knudson et al. 2007).

**Citation**

Knudson J, AU Nilekar, RT Vang, J Schnadt, EL Kunkes, JA Dumesic, M Mavrikakis, and F Besenbacher. 2007. "A Cu/Pt Near-Surface Alloy for Water-Gas-Shift Catalysis." *Journal of the American Chemical Society* 129(20):6485-6490.

## 900-MHz NMR Enables Novel Catalysis Studies

***JH Kwak,[(a)] JZ Hu,[(a)] DH Kim,[(a)] J Szanyi,[(a)] and CHF Peden[(a)]***
*(a) Pacific Northwest National Laboratory, Richland, Washington*

*γ-alumina is an important material both as a catalyst and a support to bind with other materials to form a new catalyst. When barium oxide is bound to γ-alumina, it forms a catalyst that is potentially useful in preventing pollution from diesel engines. This work discovers structural details of this complex that have been unobtainable by other techniques.*

The ability to tailor catalysts one atom at a time is a step closer to reality, in part, because of EMSL's 900-MHz nuclear magnetic resonance (NMR) spectrometer. A research team from the Institute for Interfacial Catalysis, located at the Pacific Northwest National Laboratory, used the 900-MHz NMR spectrometer to generate the highest-resolution spectra ever obtained of a common catalyst support and observed, for the first time, how the support interacts with a catalyst at the atomic scale.

To really understand catalysts, they must be studied in molecular and atomic detail. The team characterized a model system of the common γ-alumina support, γ-$Al_2O_3$, and the catalyst, barium oxide (BaO). γ-alumina materials serve as a support material for many catalysts, including BaO. Because BaO absorbs $NO_x$, a family of vehicle emissions products—the model system is a promising combination for emissions control. Despite the importance of γ-alumina materials, technology has previously not allowed detailed studies of them. The chemical properties of γ-alumina compounds are such that using traditional surface structure techniques to study them is not feasible.

The data from EMSL's 900-MHz NMR system indicates that in addition to the internal structural tetrahedral and octahedral coordinated aluminum atoms, there are also penta-coordinated aluminum atoms on the surface of the material. These atoms have different NMR relaxation times from the bulk aluminum, which is consistent with them being restricted to the surface. As BaO is added to the catalyst, the peak for these aluminum atoms becomes smaller and changes shape, showing that they are responding to the addition of the BaO. The tetrahedral and octahedral peaks do not change with the addition of BaO. Additionally, comparison of the number of BaO molecules added to the γ-alumina with the number of penta-coordinated aluminum sites that disappear in the NMR spectrum showed a nearly mole-per-mole correlation between the penta-coordinated $Al^{3+}$ ions consumed and catalyst deposited. This is strong evidence that the binding site for BaO on γ-alumina is the penta-coordinated aluminum sites. Research results are provided in detail in *Journal of Catalysis* (Kwak et al. 2007).

This work is possible only with the high sensitivity and resolution provided by the 900-MHz NMR spectrometer at EMSL.

**Citation**

Kwak JH, JZ Hu, DH Kim, J Szanyi, and CHF Peden. 2007. "Penta-Coordinated $Al^{3+}$ Ions as Preferential Nucleation Sites for BaO on γ -$Al_2O_3$: An Ultra-High Magnetic Field $^{27}Al$ MAS NMR Study." *Journal of Catalysis* 251(1):189-194.

# Microstructures of ZnO Films Deposited on (0001) and r-cut α-$Al_2O_3$ Using Metal Organic Chemical Vapor Deposition

***CM Wang[(a)], LV Saraf[(a)], and Y Qiang[(b)]***
*(a) EMSL, Richland, Washington*
*(b) University of Idaho, Moscow, Idaho*

*Detailed knowledge of the structure of oxide thin films in relation to the substrate provides researchers important tools to enable the growth of films with the desired functional properties for specific applications. Such thin film studies further EMSL's goals to characterize surfaces and interfaces with unprecedented resolution as well as to design and synthesize increasingly complex materials.*

Integrated deposition, diffraction, and microscopy resources housed at EMSL allowed researchers to study previously unknown structural details of oxide thin films that have potential applications to optoelectronics and spintronics. Earlier studies revealed differences in the qualities of zinc oxide (ZnO) films grown on different surfaces of crystalline $Al_2O_3$ – more commonly known as sapphire. EMSL users identified new and important microscopic details of the different ZnO thin film structures grown under identical conditions on $Al_2O_3$ surfaces with different crystalline orientations. Because thin film function depends on structure, such detailed characterization is a necessary step toward atomic-level design of thin films for targeted applications.

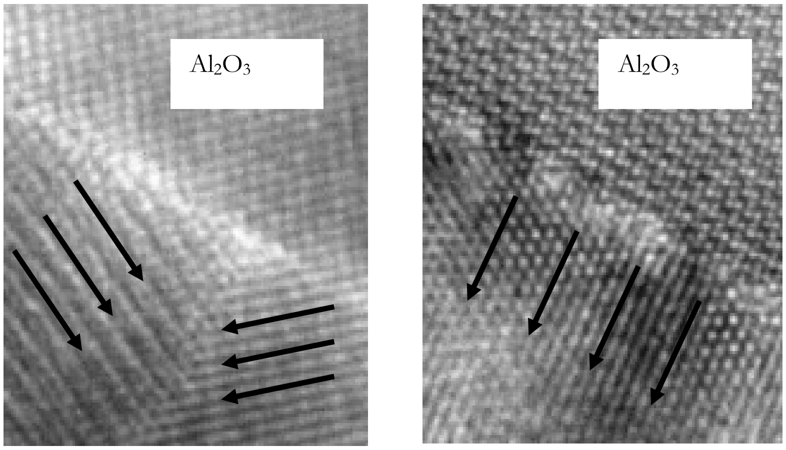


**Figure 1.** *High-resolution TEM images of portions of ZnO thin films grown on c-cut $Al_2O_3$ (left) and r-cut $Al_2O_3$ (right). Arrows indicate the prime direction of the ZnO thin film. The r-cut substrate yielded high-quality single crystals.*

For their studies, the team from the Pacific Northwest National Laboratory and University of Idaho compared thin film growth on $Al_2O_3$ cut along two different planes to yield two different ZnO bonding surfaces, referred to as c-cut and r-cut. These $Al_2O_3$ surfaces consist of the same atoms, but for each cut the arrangement of the atoms is different. Under identical conditions, these bonding surfaces were used to grow ZnO thin films with EMSL's metal organic chemical vapor deposition capability. Differences in the ZnO thin films were then characterized using high-resolution transmission electron microscopy, electron diffraction, and high-resolution TEM image simulations. This research was featured in *Thin Solid Films.*

**Citation**

Wang CM, LV Saraf, and Y Qiang. 2008. "Microstructures of ZnO Films Deposited on (0001) and r-cut α- $Al_2O_3$ Using Metal Organic Chemical Vapor Deposition." *Thin Solid Films* doi 10.1016/j.tsf.2008.04.001.

## Direct Synthesis of Nanoceria in Aqueous Polyhydroxyl Solutions

***AS Karakoti,*[(a)] *SV Kuchibhatla,*[(a,b)] *KS Babu,*[(a)] *and S. Seal*[(a,c)]**

*(a) Advanced Materials Processing and Analysis Center, University of Central Florida, Orlando, Florida*
*(b) EMSL, Richland, Washington*
*(c) Nanoscience and Technology Center, University of Central Florida, Orlando*

*One-step synthesis and stabilization of cerium oxide (ceria) nanoparticles is a most important challenge in order to efficiently use them in applications such as sensors, catalysis, and biomedical materials. This study proposes an efficient, low-cost, green chemical route to synthesize nanoceria in saccharides, while simultaneously retaining the regenerative, oxidation state switching ($Ce^{3+}$ to $Ce^{4+}$ and back) property of ceria nanoparticles. These nanoparticles are expected to have potential use in future biomedical applications such as preventing retinal damage, preventing radiation damage of healthy cells during cancer treatment, and UV absorption.*

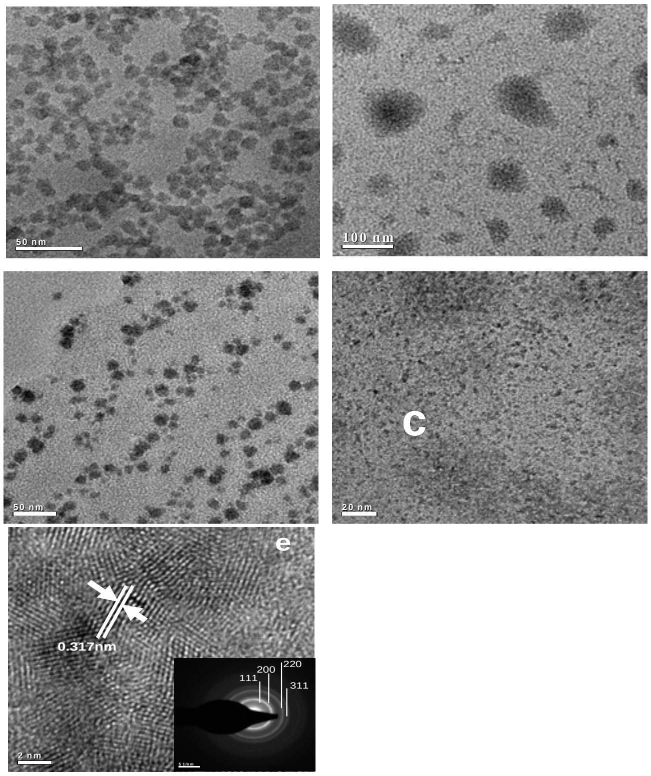
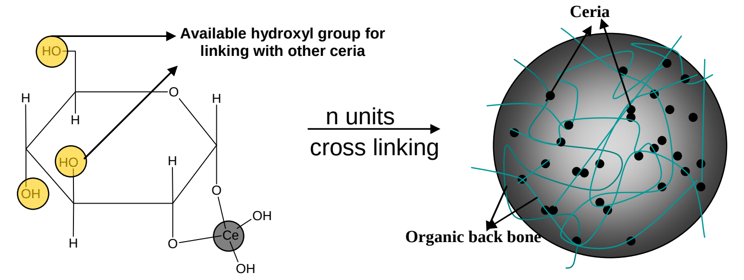


**Figure 1.** *Transmission electron micrographs for ceria synthesized in different conditions. Ceria synthesized in glucose using (a) 20-mM glucose/acid; (b) 20-mM glucose/base and in dextran; (c) 5-mM dextran/acid; and (d) 5-mM dextran/base. (e) High-resolution transmission electron microscope image and diffraction confirming the fluorite structure of ceria.*

Nanoceria has potential applications in catalysis, sensors, and biomedicine, including protecting cells again reactive oxygen species and radiation. These applications stem from cerium oxide's ability to switch oxidation states between +4 and +3, depending on the ambience (oxidizing and reducing environment). This renders nanoceria an important biomedical property for radical quenching. A whole new world of biological applications of nanoceria is opening with several interesting findings.

However, nanoceria needs to be stabilized in aqueous or non-aqueous media for all practical applications in biology. Thus, it is imperative to find a suitable delivery medium for carrying nanoceria to specific locations as an alternative route to intravenous administration. In this study, synthesis and redox chemistry of nanoceria in the presence of polyhydroxyl groups such as glucose and dextran are reported.



Ceria-saccharides complex Ceria-saccharides superstructure

***Figure 2.*** *Possible mechanism for complexation and ceria–saccharide superstructure formation.*

The effect of both acidic and basic medium on the synthesis and oxidation-state stability of nanoceria in the absence of buffer was examined using UV-visible spectroscopy and transmission electron microscopy (TEM). The basic and acidic mediums show differences in the synthesis of nanoceria in terms of size and structure without interfering with the redox chemistry. Pure and aqueous saccharides suspension of nanoceria in acid/base media undergoing redox transformation were also compared in this study.

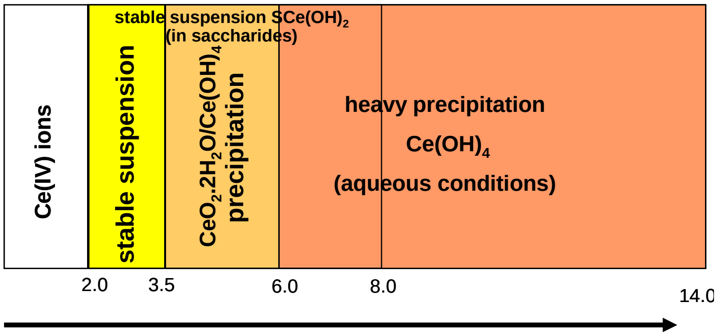


***Figure 3.*** *Precipitation behavior of cerium (IV) with respect to change in pH in oxidizing environment. The narrow stability range of ceria suspension can be extended up to a pH of 8.0 by the use of saccharides (dashed lines). Cerium is present as Ce(IV) ions (pH 0 – 2.0), stable suspension $CeO_2.2H_2O$ (pH 2.0 – 3.5), precipitate as $CeO_2.2H_2O$ (pH 3.5 – 6.0), precipitate heavily as $Ce(OH)_4$ (pH 6.0 and above), stable suspension in saccharides as S-Ce(OH)X (pH 2.0 -8.0).*

The vital points in the mechanism for engineering functionalized nanoceria are as follows:

- Ce(IV) is reduced to Ce(III) in the process of oxidation of glucose to arabinose.
- Polysaccharides have stronger tendency to complex Ce(IV) than the monosaccharides.
- Reduction of Ce(IV) to Ce(III) takes place in only highly acidic mediums (pH <2), and at this concentration no colloidal particles were detected by light-scattering photometry.

Both dextran and glucose can be used efficiently to synthesize nanoceria with enhanced stability in dextran. No significant differences were observed with respect to particle size in both dextran and glucose suspensions. However, the acidic media was found to induce higher agglomeration tendencies as compared to the basic media. Some representative TEM images are shown in Figure 1. A possible mechanism of ceria-saccharides superstructure formation by cross linking of groups due to further complexation of free hydroxyl groups of glucose with cerium(IV) is shown in Figure 2. This study clearly demonstrates that nanoceria can be synthesized directly in mono/polysaccharides by oxidizing the species in both acidic and basic environment

Importantly, the initial complex formed between cerium and sugars does not hinder the property of ceria to switch its oxidation state based on the environment. The kinetics of switching of oxidation states in solution specifically regenerated from the Ce(IV) to Ce(III) oxidation state was slower in basic medium compared to acidic medium. Moreover, from UV-visible light spectroscopy results, it is clear that the +IV oxidation state was retained in the basic medium for more than 2 months as a stable suspension, which proves the tunability of nanoceria with respect to ambience and aging. The extended stability range of ceria in saccharides over a pH range from 2.0 to 8.0 is illustrated in Figure 3.

**Citation**

Karakoti AS, S Kuchibhatla, KS Babu, and S Seal. 2007. "Direct Synthesis of Nanoceria in Aqueous Polyhydroxyl Solutions." *Journal of Physical Chemistry C* 111(46):17232-17240.

## Hidden Ferromagnetic Secondary Phases in Cobalt-Doped ZnO Epitaxial Thin Films

***TC Kaspar,[a],* T Droubay, [a] SM Heald, [b] MH Engelhard,[c] P Nachimuthu,[c] and SA Chambers[a]***

*(a) Pacific Northwest National Laboratory, Richland, Washington*
*(b) Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois*
*(c) EMSL, Richland, Washington*

*Spintronics has the potential to revolutionize electronic devices by effectively using the spin degree of freedom. However, developing the required materials necessary for room temperature operation presents a serious materials physics challenge. Investigation of potential dilute magnetic semiconductor (DMS) materials utilizing semiconducting oxide hosts was motivated by both theoretical and experimental findings of ferromagnetism at room temperature in doped oxides.*

Despite the enormous body of research that has followed, no unambiguous demonstration of carrier-mediated ferromagnetism has been made. Disparate and irreproducible experimental results have led to serious doubts as to whether the observed ferromagnetism is intrinsic to the doped oxide system or due to extrinsic effects such as contamination or phase impurity. As one example, the reported magnetization values for Co:ZnO range over two orders of magnitude (paramagnetic to $<0.05\ \mu_B$/Co to $>6\ \mu_B$/Co). Recently, our group has shown that structurally well-defined cobalt-doped ZnO is not intrinsically ferromagnetic, either in the semi-insulating state or when electronically doped *n*-type.

Weak ferromagnetism in Co:ZnO ($0.1 - 0.3\ \mu_B$/Co) has been induced by annealing in zinc vapor to diffuse interstitial zinc ($Zn_i$) into the Co:ZnO lattice. The proposed model for ferromagnetism in the presence of $Zn_i$ involves specific defect/donor formation which facilitates electron-mediated cobalt spin alignment.

In collaboration with researchers from the Advanced Photon Source at Argonne National Laboratory, researchers at Pacific Northwest National Laboratory have further explored the origin of ferromagnetism in epitaxial $Zn_i$:Co:ZnO thin films which have undergone a similar zinc vapor treatment. High-quality epitaxial $Co_xZn_{1-x}O$ thin films were deposited in EMSL by pulsed laser deposition on single crystal sapphire ($Al_2O_3$) substrates. Treatment in zinc vapor was accomplished by sealing the films in an evacuated quartz tube containing zinc metal, then heating to 600°C for 5 hours.

After the zinc vapor treatment, the films were found to be ferromagnetic at room temperature (~0.05 $\mu_B$/Co), a necessary condition for a spintronic material. Initial materials characterization by grazing-incidence x-ray diffraction and x-ray absorption near edge spectroscopy indicated that no phase segregation or cobalt reduction occurred, implying the ferromagnetism is intrinsic to $Zn_i$:Co:ZnO (Figure 1). However, when incorporating cobalt as a dopant, there is *always* the possibility of ferromagnetic secondary phase formation which can result in a weak spurious ferromagnetic signal that may be mistaken for intrinsic ferromagnetism in the doped oxide. The very weak ferromagnetism observed after zinc treatment could result if only 3 percent of the cobalt dopants formed cobalt metal precipitates; secondary phase formation at this level is below the detection limit of these sophisticated material characterization techniques.

Thus, a more careful analysis utilizing x-ray photoelectron spectroscopy at EMSL and x-ray absorption at the Advanced Photon Source was undertaken to more thoroughly investigate the possibility of cobalt metal secondary phase formation. High resolution x-ray photoelectron spectroscopy depth profiling revealed metallic cobalt in the near-surface region of the $Zn_i$:Co:ZnO film; further analysis by x-ray absorption identified the ferromagnetic secondary phase as intermetallic CoZn, which has never previously been reported in Co:ZnO. From these results, the observed ferromagnetism was shown to arise from this secondary phase, not from intrinsic ferromagnetism in $Zn_i$:Co:ZnO. This work emphasizes the vigilance required in materials characterization before intrinsic ferromagnetism can be definitively attributed to the substitutionally doped oxide phase.

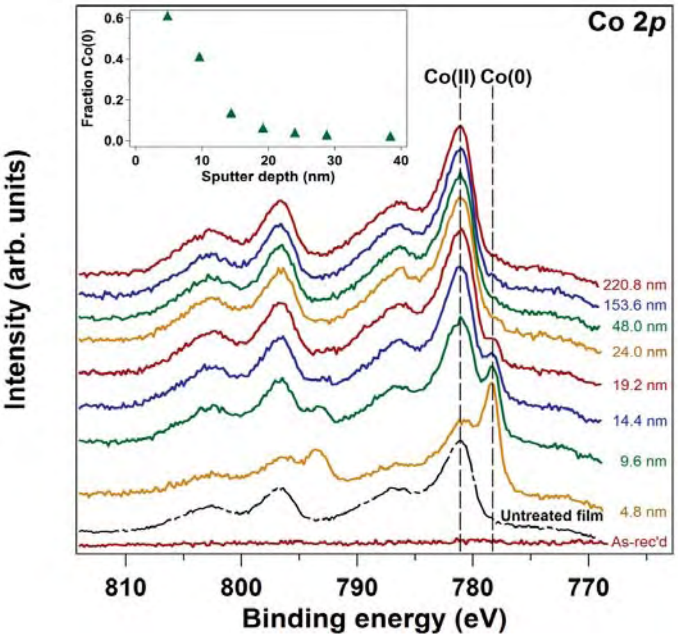


***Figure 1.*** *X-ray photoelectron spectroscopy depth profiles of 310 nm a-*$Co_{0.1}Zn_{0.9}O$ *after zinc treatment. For comparison, the cobalt 2p spectrum of an untreated film after one sputter cycle is shown (dash-dot line). Inset: fraction of cobalt present as Co(0) as a function of depth in* $Zn_i$*:Co:ZnO, as determined by fitting the x-ray photoelectron spectroscopy cobalt 2p spectra.*

This work was published in *Physical Review B* as a Rapid Communication and was subsequently selected as a research highlight by *Nature Materials* [7(7):517].

**Citation**

Kaspar TC, T Droubay, SM Heald, MH Engelhard, P Nachimuthu, and SA Chambers. 2008. "Hidden Ferromagnetic Secondary Phases in Cobalt-Doped ZnO Epitaxial Thin Films." *Physical Review B* 77(20):201303.

## Alcohol Chemistry on Rutile $TiO_2$(110): The Influence of Alkyl Substituents on Reactivity and Selectivity

***YK Kim,[(a)] BD Kay,[(b)] JM White,[(a)] and Z Dohnàlek[(a)]***

*(a) University of Texas at Austin, Austin, Texas*
*(b) Pacific Northwest National Laboratory, Richland, Washington*

*$TiO_2$ is widely used as a catalyst and may provide a pathway for the use of solar radiation as a viable source of clean energy. This work is a detailed study of the reaction mechanisms for the dehydrogenation reaction of alcohols on $TiO_2$(110). This knowledge will increase our fundamental understanding of elementary surface reactions and may lead to improvements and new applications in heterogeneous catalysis.*

Many reactions on solid surfaces (e.g., oxides) occur on defect sites. On prototypical rutile $TiO_2$(110) surfaces, there is direct scanning tunneling microscopy (STM) evidence that bridge bonded oxygen vacancies (BBOVs) are sites for dissociation of oxygen, water, and alcohols. In the surface science and catalysis literature involving alcohol, chemistry on $TiO_2$, dehydration to alkenes above 500 K is well established while dehydrogenation to aldehydes or ketones and reformation of the dosed alcohols are less well established. The chemical pathways leading to these products are typically described terms of paths requiring BBOVs. However, the inability to control surface order and BBOV concentration may account for reported variations in temperature-programmed desorption (TPD) profiles of alcohol dehydration, making it difficult to establish unambiguous connections between catalytic dehydration activity and the local surface structure of $TiO_2$(110).

As part of a research program to establish direct atomic-level descriptions by combining STM and reaction rate measurements for oxygenates on oxides, we have recently reported on the ensemble average surface chemistry of three different isotopically labeled 2-propanols dosed at 100 K on $TiO_2$(110). For the first time, a low-temperature (LT) dehydrogenation path (300-450 K) was found to accompany the well-established high-temperature (HT) path ($T > 450$ K). While surface structure is one key, variations with the alcohol are also expected and have been reported; while dehydration typically dominates, dehydrogenation contributes more for primary alcohols. The present study was motivated by a desire to determine the detailed roles played by the alkyl substituents on the accessibility of the LT and HT channels and on the dehydration selectivity. The inductive and steric effects of alkyl substituents are the concepts commonly used to understand the trends in the reactivity of similar molecules in homogeneous organic chemistry (e.g., in liquids). Here, we show that similar concepts can be successfully applied to understand the heterogeneous reactions at gas-solid interfaces. In this work, we report the details of the LT and HT reaction paths for primary, secondary, and tertiary alcohols for 100 K doses on well-ordered TiO$_2$(110) with a reproducible, relatively small BBOV concentration (3.5%).

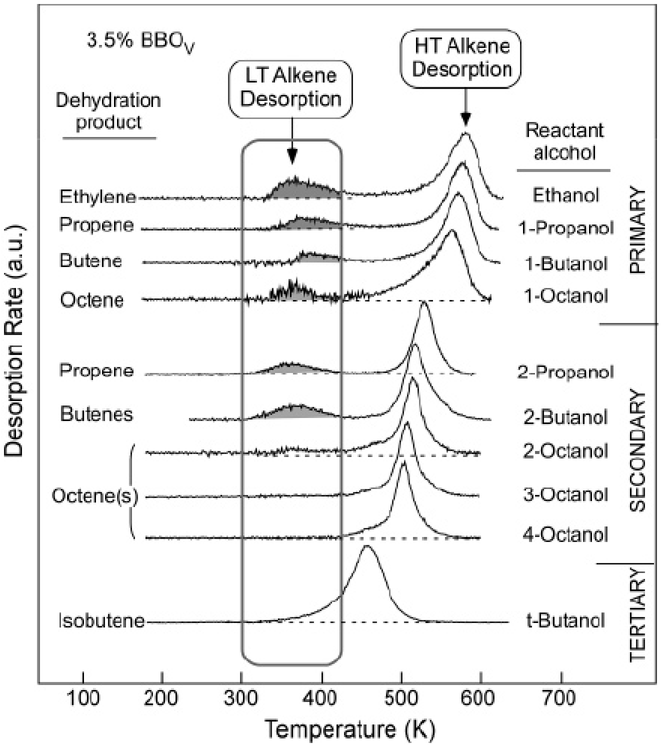


***Figure 1.*** *TPD spectra of alkenes from 10 alcohols dosed on* $TiO_2^-$*(110) at 100 K grouped as primary, secondary, and tertiary. The net alkene desorption spectra (shown) were obtained by subtracting the fragmentation contributions of molecular alcohol. The 27 and 41 amu were used for ethylene and propene, respectively, and 56 amu was used for butenes and octenes. The alcohol dose was set to 1 ML, and all spectra were normalized to the HT alkene desorption peaks.*

With the above picture in mind, Figure 1 displays the alkene TPD spectra for 1 ML of 10 different alcohols deposited on TiO$_2$(110). In the LT region, seven of the 10 (ethanol, 1- and 2-propanol, 1- and 2-butanol, and 1- and 2-octanol) exhibit intensity, whereas the other three (3- and 4-octanol, and *t*-butanol) do not. When the LT channel is present, the peak temperature shows no systematic variation with alcohol structure. On the other hand, the HT channel is observed for all 10 alcohols and varies systematically with two properties of the dosed alcohol. First, the HT peak positions group together; primary alcohols are systematically higher by 50-60 K than the secondary alcohols which are, in turn, higher by another 50-60 K than the tertiary alcohol. Within each grouping, the production rate maximum drops 10-20 K as the chain lengths increase. The HT shifts are explained in terms of inductive electronic effects of the alkyl groups; the latter are described empirically using the Taft parameters of organic reaction chemistry.

The variations in LT alkene production confirm effects related to the number of carbon atoms in the alkyl chains. For primary alcohols. the low-temperature channel is active for all chain lengths studied (up to C8). For *t*-butanol, there is no evidence for LT alkene production. For secondary alcohols, alkene production is observed, except if there is no CH$_3$ attached to the alpha carbon.

Based on a series of experiments, we have developed a mechanism for the LT reaction pathway. The LT dehydration pathway is attributed to the species bound to $Ti^{4+}$ rows. Mobility of ROH along the $Ti^{4+}$ rows is expected and was observed in STM below the temperature where this desorption commences. The mechanism, illustrated in Figure 2, involves a mobile and oriented, but undissociated, alcohol molecule that undergoes a 1D random walk along a given $Ti^{4+}$ row (Step I). An encounter with 2-propoxy, also oriented, during this 1D random walk form a critical activated complex (Step II) that rearranges in the LT region to form propene and 2-propanol that desorb and a mobile OH group bound to $Ti^{4+}$ (Step III), $HO_{Ti}$. Finally, in the OH groups, one on a BBO row, $HO_{bb}$, and the other mobile and on an adjacent $Ti^{4+}$ row, $HO_{Ti}$, collide and form $H_2O$ that desorbs leaving the $O_{bb}$. Thus, no net loss of lattice oxygen occurs during the reaction cycle.

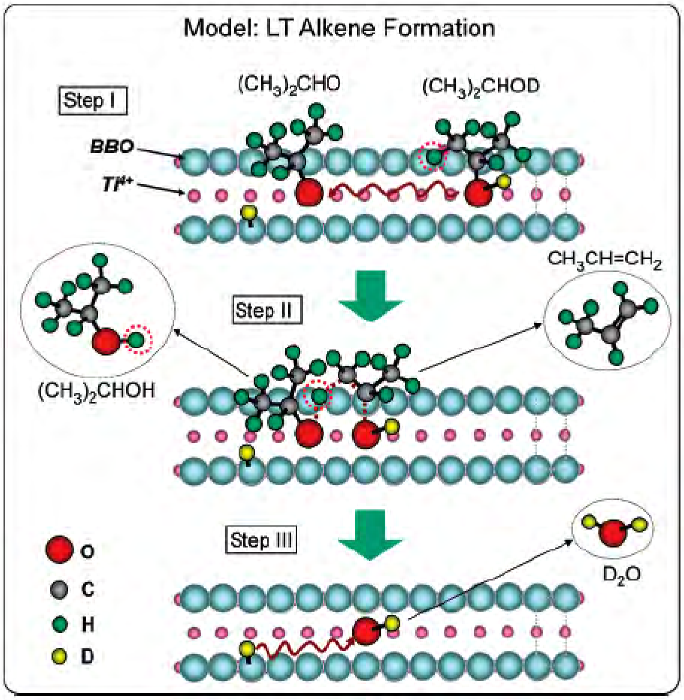


***Figure 2.*** *Schematic of proposed LT dehydration mechanism. The key intermediate is a complex (Step II) formed by interaction of an oriented alkoxide with an oriented chemisorbed alcohol (Step I). There is a concerted rearrangement that involves beta-H, in the case shown on* $CH_3$*, coupling to the alkoxide oxygen and simultaneous cleavage of the C-O bond of the chemisorbed alcohol. Step III illustrates the final recombinative desorption of* $D_2O$*.*

The exact nature of the activated complex is not clear, but the experimental evidence suggests that it requires two oriented reactants with close proximity of their alpha and beta carbon atoms. Details of this exciting research were published in the *Journal of Physical Chemistry C.*

**Citation:**

Kim YK, BD Kay, JM White, and Z Dohnalek. 2007. “Alcohol Chemistry on Rutile $TiO_2(110)$: The Influence of Alkyl Substituents on Reactivity and Selectivity.” *Journal of Physical Chemistry C* 111(49):18236-18242.

# Conductivity of Oriented Samaria-Doped Ceria Thin Films Grown by Oxygen-Plasma-Assisted Molecular Beam Epitaxy

***ZQ Yu,[(a)] SV Kuchibhatla,[(b)(c)] LV Saraf,[(b)] OA Marina,[(d)] CM Wang,[(b)] MH Engelhard,[(b)] V Shutthanandan,[(b)] P Nachimuthu,[(b)] and S Thevuthasan[(b)]***

*(a) Nanjing Normal University, Nanjing, China*
*(b) EMSL, Richland, Washington*
*(c) University of Central Florida, Orlando, Florida*
*(d) Pacific Northwest National Laboratory, Richland, Washington*

*Due to global demands for increased energy resources and sustainable and renewable alternative energy, technologies such as solid-oxide fuel cells (SOFCs) are becoming the significant focus of researchers across the globe. In an effort to make this technology economically and practically viable for everyday use, it is of paramount importance for researchers to understand the fundamental aspects that control the performance of an SOFC. The heart of the SOFC is the electrolyte material that transports oxygen ions from cathode to anode. High-quality, epitaxial thin films of doped cerium oxide (a potential material for SOFC electrolytes at low and intermediate temperatures) are an excellent resource that allows researchers to explore the fundamental mechanisms that control the ionic conduction in SOFC electrolytes.*

With the increasing demand for energy efficiency and the realization that greenhouse gas emissions must be reduced, technologies such as solid-oxide fuel cells (SOFC) are gaining significant attention. The fundamental understanding of the actual mechanisms that govern the ionic conduction in SOFC electrolytes is still elusive. A major hurdle in overcoming this bottleneck stems from the lack of studies based on high-quality materials. Use of conventional powder-processed pellets with porosity and grain boundaries makes analysis more complicated. Oxygen-plasma-assisted molecular beam epitaxy capabilities housed at EMSL have allowed researchers to synthesize high-quality epitaxial thin films with controlled dopant levels and thickness. Among the various materials used for low- and intermediate-temperature SOFC electrolyte application, samaria ($Sm_2O_3$, samarium oxide) doped ceria

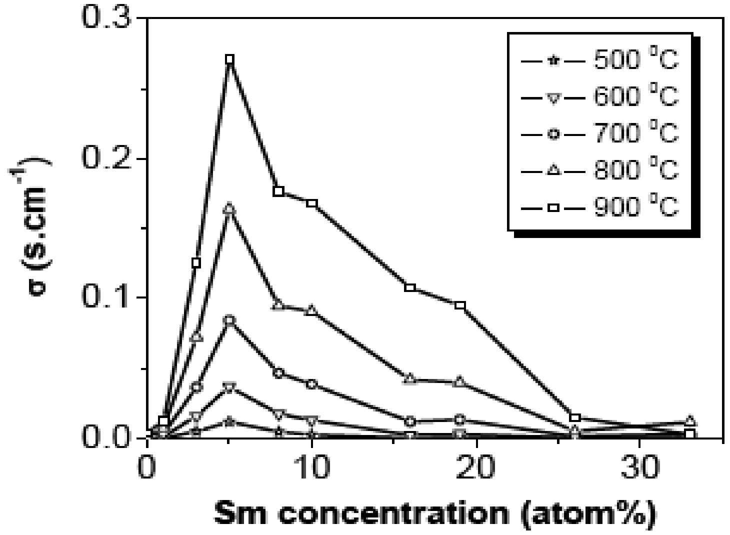


***Figure 1.** The conductivity of Ce1-xSMxO2*Δ films as a function of samaria concentration for the temperature range of 500-900°C.*

($CeO_2$, cerium oxide) (SDC) is expected to be the best possible material. Hence, high-quality epitaxial SDC films were grown on sapphire (0001) substrates.

The grown films were characterized using various *in-situ* and *ex-situ* techniques to understand their structure, crystalline quality, elemental distribution, and chemical composition (oxidation states of the cations). After establishing the optimum growth conditions, films with various amounts of dopant concentrations were grown (1 – 33 atom % samaria). Electrochemical impedance measurements were carried on these films using a four-probe van der Pauw method. The conductivity data obtained from these measurements were analyzed as a function of temperature and dopant concentration (Figure 1). Some of the salient features from this work are highlighted below:

- Ceria films with more than 10 atom% samaria were found to show polycrystalline features, while the films with less than 10 atom% samaria were found to be epitaxial, highly oriented films.
- Rutherford backscattering spectrometry and x-ray and electron diffraction measurements confirmed the high-quality, epitaxial nature of the films.

- 5 atom % samaria doping was found as an optimum concentration to obtain maximum conductance among various compositions.
- The reduction in the conductivity in films with high dopant concentration is attributed to the polycrystalline nature of the films. In the polycrystalline films, grain boundaries may act as scattering centers for the oxygen ions, hence the observed decrease in the overall conductivity.
- The higher ionic conduction at lower temperatures in the highly oriented SDC films is attributed to the alignment of oxygen vacancies [generated to retain the electrical neutrality of the ceria ($Ce^{4+}O^{2-}$) crystal when doped with $Sm^{3+}$]. The aligned oxygen vacancies help efficiently transport oxygen ions across the electrolyte from cathode to anode.

Various ongoing user research programs at EMSL are focused on exploring the finer details behind these observations and are aimed at developing a comprehensive understanding of the fundamental mechanisms that control the performance of nanoscale doped-oxide materials as potential SOFC electrolyte materials. This research was published in *Electrochemical and Solid State Letters* (Yu et al. 2008).

**Citation:**

Yu ZQ, SV Kuchibhatla, LV Saraf, OA Marina, CM Wang, MH Engelhard, V Shutthanandan, P Nachimuthu, and S Thevuthasan. 2008. "Conductivity of Oriented Samaria-Doped Ceria Thin Films Grown by Oxygen-Plasma-Assisted Molecular Beam Epitaxy." *Electrochemical and Solid State Letters* 11(5):B76-B78.

# Laser and Electrical Current Induced Phase Transformation of $In_2Se_3$ Semiconductor Thin Film on Si(111)

**CY Lu,[a] PJ Shamberger, [a] EN Yitamben, [a] KM Beck,[b] AG Joly,[c] MA Olmstead,[a] and FS Ohuchi[a]**

*(a) University of Washington, Seattle, Washington*
*(b) EMSL, Richland, Washington*
*(c) Pacific Northwest National Laboratory, Richland, Washington*

*Materials with rapid and reversible switching between amorphous and crystalline phases, and which exhibit significant electrical resistivity or optical reflectivity change between these phases, are promising candidates for phase-change non-volatile memory. The strong change in optical reflectivity during the amorphous-crystalline phase transition is the basis of re-writeable compact disk and digital video disk technology. During the past decade, binary chalcogenide semiconductors such as InSe/GaSe and $In_2Se_3$ have been investigated as potential phase-change media in proposed data storage and memory devices. This research investigates the phase-change mechanisms of $In_2Se_3$ using EMSL's photoemission electron microscope capability. This research will be highlighted in a journal article published this summer in* Applied Physics A.

The electrical resistivity of $In_2Se_3$ increases by a factor of $10^5$ from the crystalline to the amorphous state. However, the structural details of phase-change in $In_2Se_3$ films on silicon and the energetic requirements for phase change have not been fully explored. $In_2Se_3$ exhibits a complex phase system in which various structures with different arrangements of inherent defects can form. This complexity originates from many energetically similar routes by which trivalent and divalent atoms can combine to satisfy their bonding requirements and leads to several crystalline phases with the same $In_2Se_3$ stoichiometry.

This research analyzes the crystallization and amorphization of $In_2Se_3$ thin films on Si(111) (~ 30 nm thick) via resistive heating and laser annealing, respectively. The initially amorphous films were crystallized using resistive heating (time-scale of several seconds), while a 150-micron-diameter spot was re-amorphized using nanosecond laser annealing. The film morphology and conductivity were probed with scanning tunneling microscopy and photoelectron emission microscopy (PEEM), the crystallinity was probed with x-ray diffraction and low-energy electron diffraction, and the stoichiometry with Rutherford back-scattering spectroscopy. The stoichiometry, morphology, and crystal structure of the crystallized $In_2Se_3$ film and its orientation with respect to the substrate are determined.

The EMSL PEEM was equipped with both Hg ($h\nu = 5.1$ eV) and $D_2$ ($h\nu = 6.0$ eV) sources for imaging a 150-μm-diameter region of the sample. An Nd:YAG laser ($\lambda = 266$ nm, $h\nu = 4.7$ eV, FWHM pulse width 20 ns, spot diameter 100 μm, 0.1 mJ/pulse at 1 Hz repetition rate) was interfaced to the PEEM and used to amorphize the crystalline film. The laser is introduced through an ultraviolet-grade-fused silica window to the PEEM objective chamber holding the sample.

While a slow anneal below the melting temperature can lead to crystallization of an amorphous film, returning to the amorphous state requires rapid heating and cooling to quench in the disordered state. This was accomplished with pulsed laser annealing. The sample was monitored with the PEEM, which distinguishes structures on the surface through a combination of their work function, electrical conductivity, and density of states near the Fermi level.

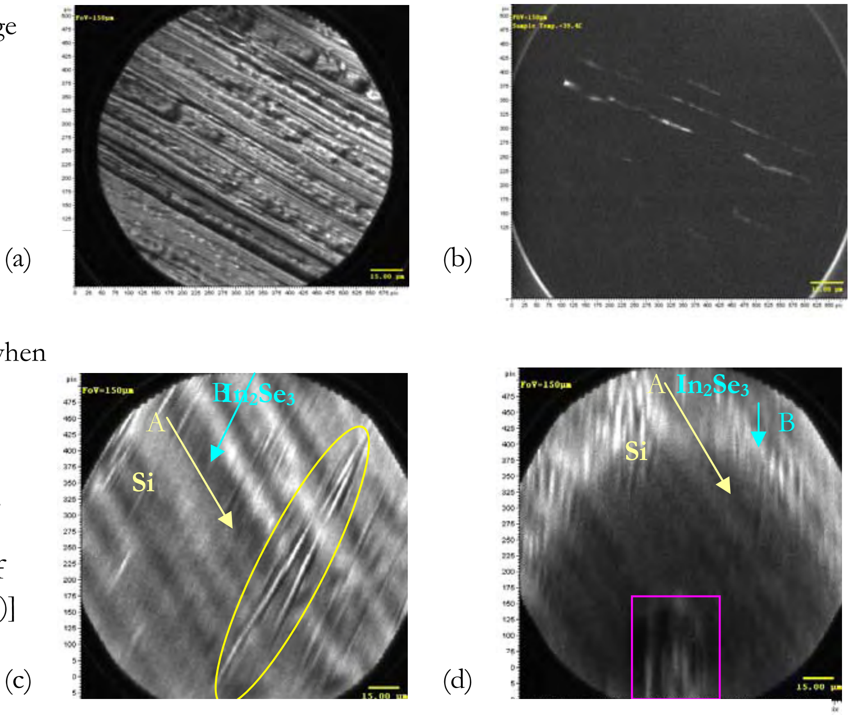


**Figure 1.** *PEEM images (field of view 150 µm, scale bar 30 µm) for (a) clean Si(111); (b) amorphous $In_2Se_3$ film on Si(111); (c) annealed $In_2Se_3$/Si(111); (d) after irradiation with 266-nm photon pulse. Images presented here are acquired with mercury lamp illumination (hν = 5.1 eV).*

Figure 1(a) shows a PEEM image of a clean Si(111) substrate after being argon-sputtered and then annealed around 850°C. An amorphous $In_2Se_3$/Si(111) film deposited is shown in Figure 1(b). The room-temperature-deposited $In_2Se_3$ film presents a completely dark PEEM image when using either the mercury lamp (5.1eV) or $D_2$ lamp (6.0 eV), except for defect lines running through the center of the image.

A PEEM image was obtained of the same film before [Figure 1(c)] and after [Figure 1(d)] laser annealing. Similar results were obtained with both mercury and $D_2$ illumination, although only the mercury results are shown. Comparison to silicon substrates without $In_2Se_3$ films [Figure 1(a)] indicates that the wider stripe structure running from upper left to lower right arises from the underlying silicon terrace structure (yellow arrows), while the narrower lines (blue arrows) correspond to the texture of the $In_2Se_3$ films. Two crossed lines marked in the oval are defects on the surface.

The 266-nm laser was used to anneal a spot on the sample approximately 150 microns in diameter near the place where the image in Figure 1(c) was taken., Single pulses of 0.1-mJ and 20-ns duration were measured at the laser head. Subsequent aperture-reduction and focusing culminated in a final pulse fluence of < 50 mJ/cm$^2$. The resulting annealed region is shown in Figure 1(d), where a dark circular region may be observed surrounded by features characteristic of the crystalline $In_2Se_3$ film. The darker region still shows (though with less contrast) the structure characteristic of the underlying silicon substrate, with $In_2Se_3$ features less distinct.

The contrast between the crystalline and amorphous regions in the PEEM could arise from differences in work function, in densities of states near the Fermi level, or in film conductivity. The work function of crystalline $In_2Se_3$ is 4.35eV, so both mercury (5.1 eV) and $D_2$ (6.0 eV) illumination should result in electron emission. Our photoemission measurements on a 1-nm-thick film show an In 4d core level shift of ~ 0.7 eV to higher binding energy (relative to the Fermi energy) from the amorphous to the annealed phase, while the silicon 2p shifts by only 0.1 eV in the same direction. If the In shift were completely due to a change in work function, then the mercury radiation would be close to threshold for photoemission, but there should still be significant emission with $D_2$ radiation. However, we find no emission with either source for the as-deposited film except at large-scale defects [Figure 1(b)]. It is thus likely that photoexcited electrons become trapped in the highly resistive amorphous material and cannot travel to the surface for emission into vacuum.

The control of material phase (amorphous, or one of several possible crystalline or polycrystalline states) is essential to the properties of modern devices. The difference in properties associated with a phase change may be exploited for device operations, as in DVDs where the change in optical reflectivity between crystalline and amorphous states allows media rendition. Driven by the need for a new paradigm to continue the relentless increase in both density and speed that has characterized developments in computer memory for four decades, one promising avenue for non-volatile memory is phase-change non-volatile memory, for which chalcogenides are prime candidates.

Amorphous-crystalline phase transitions can be achieved by applying voltage pulses with different amplitudes and durations in the range of tenths of nanoseconds. In our study, we have shown that rapid, selective, and local crystal-amorphous transformation can be realized using pulsed, ultraviolet nanosecond lasers at low fluences. This is a necessary step in the development of high-density/high-speed chalcogenides-based optical phase-change non-volatile memory.

## A Fast Analysis Technique to Evaluate Scintillation Response

***Y Zhang[a], M Elfman[b], BD Milbrath,[c] and WJ Weber[c]***

*(a) EMSL, Richland, Washington*
*(b) Lund Institute of Technology, Lund, Sweden*
*(c) Pacific Northwest National Laboratory, Richland, Washington*

*Demands for national security, medical physics, and high-energy nuclear physics applications have prompted research efforts for both improved performance of materials for radiation detection and accelerated materials discover (van Eijk 2003). Existing detector materials do not meet the increasing requirements of nuclear nonproliferation and homeland security applications. Next-generation radiation detector materials with excellent energy resolution at room temperature are needed. Both accelerated materials discovery and efficient techniques that can investigate material properties relevant to detector performance are required.*

For gamma ray (γ-ray) detection, a relatively large high-quality crystal is needed for complete absorption of γ-ray energies of interests. New materials discovery has been limited due to the difficulties inherent to large crystal growth; whereas high-quality thin films of candidate materials can be readily produced by various modern deposition techniques. Charged particles, such as $He^+$, can easily deposit all their energy within a few tens of micrometers, and the corresponding scintillation response can be used to characterize material properties relevant to detector performance. In the current study, a fast screen technique, applicable to thin films or small crystals, is demonstrated to provide the scintillation response of the materials, where energetic ions are used instead of gamma rays. Benchmark materials of bismuth germanate (BGO, $Bi_4Ge_3O_{12}$) and europium-doped calcium fluoride ($CaF_2$:Eu) crystals are chosen to demonstrate the ion approach.

### *Experimental Procedures*

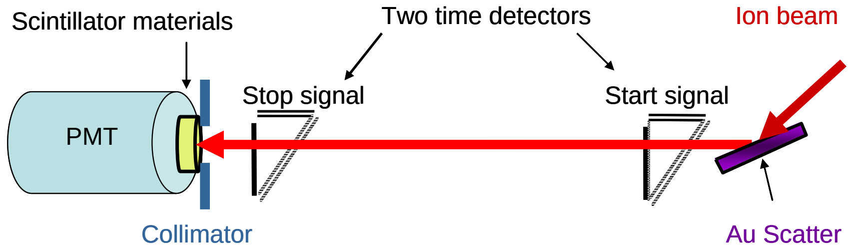


***Figure 1.*** *Schematic drawing of the TOF-scintillator-PMT setup for the scintillation measurement, where BGO or $CaF_2$:Eu is mounted between the second time detector and the PMT.*

The scintillation response of materials to $He^+$ was measured using a time-of-flight (TOF) setup. $He^+$ ions with energy of 3.5 MeV were produced using a forward scatter method, as shown in Figure 1. Monogenic particles of helium were produced by an NEC tandem accelerator and forward scattered at 45 degrees to the primary beam direction into the TOF telescope by a bulk gold target. Using the forward scatter method, energetic $He^+$ particles were produced over a continuous range of energies from a few tens of keV to a few MeV, so the scintillation response could be investigated over a continuous energy range.

## Results and Discussion

### *Energy Resolution*

To demonstrate that the current approach that can be used as a fast screening technique, the scintillation response of both BGO and $CaF_2$:Eu was examined, and the results are shown in Figure. 2. With superior energy resolution and fast response of the TOF telescope, the energy of individual particles before impinging on the scintillating crystal were determined with a high counting rate. In about 30 minutes, more than 1 million particles were detected by both the $CaF_2$:Eu crystal and the TOF telescope in a coincident mode, which allows quantitative analysis of material performance over a continuous energy range in a relatively short time.

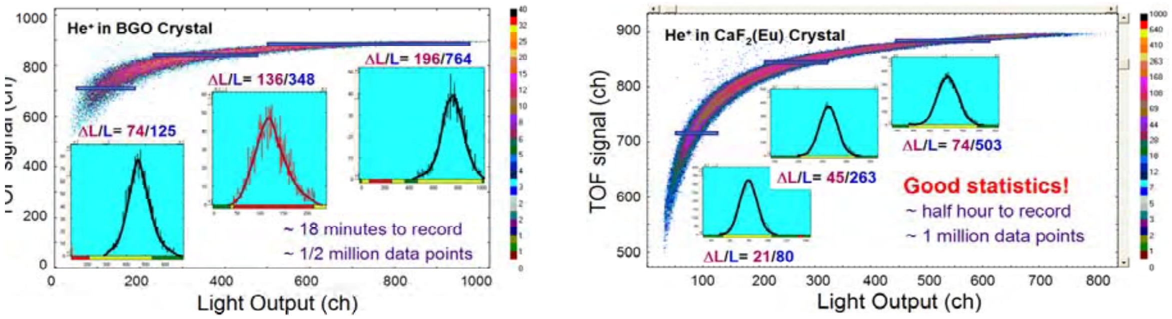


***Figure 2***. *TOF versus light output of BGO (left) and $CaF_2$:Eu (right) to $He^+$ particles. The insets are the light output profile of the particle at TOF=715, 840 and 885, respectively. The light intensity is governed by the peak position L and the energy resolution can be determined by ΔL/L as shown by the three insets.*

TABLE I

FAST ESTIMATION OF ENERGY RESOLUTION (ΔL/L) OF SCINTILLATION RESPONSE

| TOF (ch) | BGO | $CaF_2$:Eu |
|---|---|---|
| 715 | 59% | 26% |
| *840* | 39% | 17% |
| *885* | 26% | 15% |

The measured energy resolution in the current study is defined as the full width at half maximum (FWHM) of the peak normalized to its energy (ΔL/L). Fast determination of energy resolution of scintillation response can be obtained by online analysis, as shown by the three examples with corresponding ΔL/L values in Table 1 and Figure 2. Compared with the BGO crystal, the $CaF_2$:Eu crystal indicates a much better energy resolution, as demonstrated by the examples at three energies (different TOF).

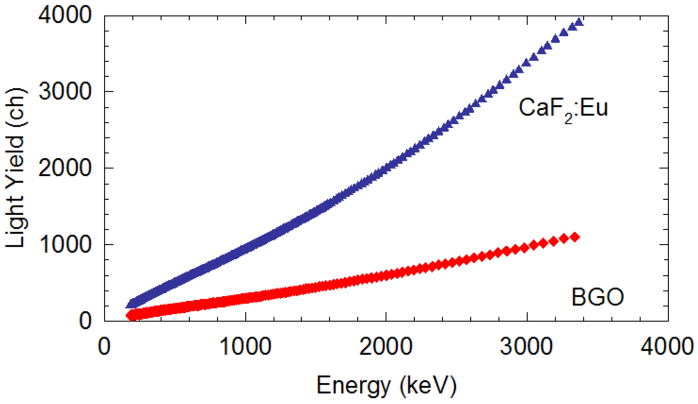


***Figure 3.*** *Light yield (L) as a function of particle energy (E) for $CaF_2$:Eu and BGO from a similar experimental setup.*

### *Light Yield*

Absolute light yield is one of the critical properties when evaluating a scintillation material. The scintillator light yield in this study is given by the pulse height (related to the number of photons) measured due to the total energy deposition of the impinging particles. The scintillation response of the two crystals was measured over the energy range from about 100 keV to approximately 3400 keV using the current technique. As shown in Figure 3, much higher light yield is observed for $CaF_2$:Eu, as compared with BGO. The relative ratio is in good agreements with the literature value from gamma ray measurements, where the absolute light yield is 8,200 and 24,000 photons/MeV for BGO and $CaF_2$:Eu, respectively (Knoll 2000; Holl et al. 1988).

### *Conclusion*

For fast screening purposes, the candidates of radiation detector materials can be simply investigated using readily available energetic ions, such as hydrogen or helium ions. The measured light yield and energy resolution observed in the candidate scintillation materials can be compared with the results from benchmarked detector materials. This approach can be applied as a fast analysis technique to assist current efforts on the discovery of new radiation detection materials. The primary assumption is that thin-film materials or small crystals, whose energy resolution to alphas is poor, are unlikely candidates for gamma detectors, while materials that demonstrate good detector response are candidate materials for further investigation, including large crystal growth.

Furthermore, the use of charged particles to deposit energy provides additional control and separation of mechanisms related to photon response and transport properties. This work demonstrates a possible pathway to achieve fundamental understanding of charged particle response and energy resolution, which may provide insight into the different mechanisms that govern the scintillation processes and the origins of light yield nonlinearity in different materials.

### Citations

Holl I, E Lorenz, and G Mageras. 1988. “A Measurement of the Light Yield of Common Inorganic Scintillators.” *IEEE Transactions on Nuclear Science* 35(1):105-109.

Knoll GF. 2000. *Radiation Detection and Measurement. John Wiley Wiley and Sons*, *Inc.*

van Eijk CWE. 2003. “Inorganic Scintillators in Medical Imaging Detectors.” *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment.* 509(1-3):17-25.

Wang CM, LV Saraf, TL Hubler, and P Nachimuthu. 2008. "Tilted Domain Growth of Metalorganic Chemical Vapor (MOCVD)-Grown ZnO(0001) on α-$Al_2O_3$(0001)." *Journal of Materials Research* 23(1):13-17.

# Enhanced Understanding of Titania's Catalytic Mechanism through Computational Modeling

***S Kerisit[a], NA Deskins[a], KM Rosso[a], M Dupuis[a]***

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

*Using EMSL's computational modeling capabilities, fundamental insight into the properties of titania surfaces is obtained, which is knowledge necessary for understanding the potential use of titania-based catalyst for providing a source of hydrogen fuel and a the potential for aiding in Hanford Site cleanup.*

Since the dawn of time, mankind has been driven to obtain both energy and an understanding of where this energy came from, and more importantly how to control it. While early mankind only had fire and little understanding, modern man has a multitude of energy choice with more choices on the horizon. Unfortunately, even though the world's economy is driven by energy, understanding is does not always keep up with these advances, and without understanding we will not be able to make the right choices as a nation or as individuals.

Recently, hydrogen has gained much attention as an environmentally friendly energy medium. Titania ($TiO_2$) has been the subject of extensive research because of its potential use as a catalyst for the production of hydrogen via water splitting. For example, experimentalist have already shown that trimethylacetic acid can be decomposed into isobutene and carbon dioxide on titania, but the theoretical models are not advanced enough to explain the fundamental interactions. In the dynamic realm of condensed phase chemistry, the formation and stability of bonds is controlled by geometry, temperature, and pressure. Probing these aspects provides fundamental insight, which leads to an understanding of bonding preferences that could eventually be exploited to manipulate catalytic behavior, and thus custom catalysts.

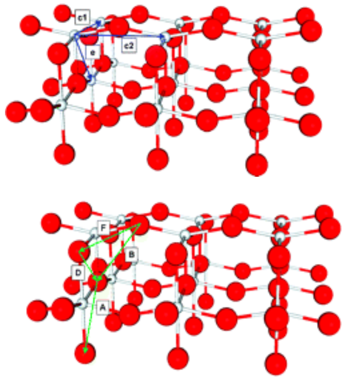


***Figure 1.*** *Electron (top) and hole (bottom) polaron transfer directions at the anatase (001) surfaces.*

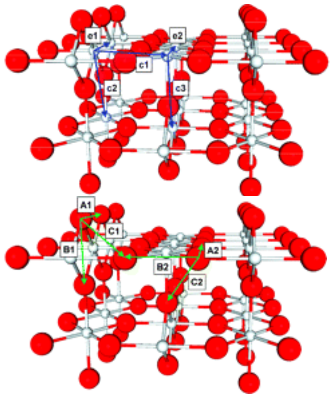


***Figure 2****. Electron (top) and hole (bottom) polaron transfer directions at the rutile (110) surface.*

Scientists at Pacific Northwest National Laboratory have teamed up to understand the nature of the chemical reactivity of titania. Using EMSL's supercomputer, these researchers were able to obtain good agreement with experimental results and new insight into the underlying chemistry. This extensive study was recently published in the American Chemical Society's high-ranking *Journal of Physical Chemistry C.*

The transport of electrons and holes (i.e., the hole left when an electron moves) in titania is well described with a polaron model. Polarons are quasi-particles that consist of an electron or hole and the resulting lattice polarization. In titania, a electron polaron is localized on a titanium site, thereby reducing it to $Ti_3^+$, whereas a hole polaron is located on the oxygen site, thereby oxidizing it to $O^-$. Polarons interact strongly with vibrations and lower their energy by creating a local distortion of the lattice. Polarons can be so small that the distortion is smaller than a lattice constant. Polaron transfer in titania is described by a model whereby the reactants (before charge transfer) and products (after charge transfer) potential-energy surfaces are assumed to be parabolic with respect to the reaction coordinate. As the titania is heated, the atoms vibrate more. These thermal fluctuations allow the reactants and products states to interchange freely (i.e. they are energetically degenerate). Such interactions fundamentally change the nature of the material.

The first step in studying polarons was to develop potential parameters for titania based upon energies obtained from density functional theory calculations. These parameters were validated against the extent of lattice distortion of titania crystal lattices upon introduction of electron and hole polarons and the difference in polaron formation energies between rutile and anatase. Good agreement was obtained throughout, and electron polarons have a greater intrinsic affinity for the anatase phase, whereas hole polarons favor the rutile phase. The newly derived potential model was employed in a series of molecular dynamics simulations to investigate the surface effects on the energetics of polaron transfer using the rutile (110) and anatase (001) surfaces. Both the reorganization energy and free energy as a function of depth indicate that the surface effects are limited to the first couple of surface layers at most. However, the topmost surface layer shows large deviations from bulk behavior with increases in reorganization energy varying from approximately 5 to 25 percent and free energies of surface sites up to 3 eV higher than equivalent bulk sites. Polaron transfer directions on the surface are presented in Figures 1 and 2. Although the polaron free energy increases as it approaches the surface, the electrostatic potential of some subsurface sites can be significantly lower than that of equivalent sites in the bulk and thus act as traps for diffusing polarons, as was found for hole polarons at the rutile (110) surface. The presence of these sites may have important implications for the availability of electrons and holes in photocatalytic reactions.

The implications of these discoveries extend beyond just beyond understanding for future energy developments. Titania has also been proposed as a catalyst for the degradation of organic pollutants. The production of nuclear materials has resulted in the release of organic contaminants into the environment at DOE sites. Obtaining an understanding of catalysts that will break down contaminants is a major challenge to the cleanup mission.

### Citation

S Kerisit, NA Deskins, KM Rosso, and M Dupuis. 2008. "A Shell Model for Atomistic Simulation of Charge Transfer in Titania" *Journal of Physical Chemistry C* 112: 7678–768.

# Fiscal Year 2008 User Projects

**3D Imaging of Organic Nanoparticle Fillers in Organic Matrices**
J Simonsen, Oregon State University, Corvallis, Oregon

**3-Dimensional Reconstruction and Modeling of Bacterial Extracellular Polymeric Substances (ExPS)**
MJ Marshall, Pacific Northwest National Laboratory, Richland, Washington
A Dohnalkova, EMSL, Richland, Washington

**$^{13}$C NMR Investigation of Occluded Carbonate in Aluminum (Oxy)Hydroxides**
JR Rustad, University of California, Davis, Davis, California
J Boily, Umea University, Umea, Sweden
DA Dixon, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**$^{43}$Ca NMR Spectroscopy of $Ca^{2+}$ Dependent Proteins and Models**
AS Lipton, PD Ellis, R Heck, Pacific Northwest National Laboratory, Richland, Washington
JV Hanna, ANSTO, Menai N.S.W., Australia

**$^{51}$V Solid-State MAS NMR Studies of Vanadium Haloperoxidases**
S Bolte, KJ Ooms, TE Polenova, University of Delaware, Newark, Delaware

**$^{103}$Rh and $^{13}$C NMR Studies of Rh Complexes used to Catalyze the Oxidative Carbonylation of Toluene to Toluic Acid**
JJ Zakzeski, AT Bell, University of California, Berkeley, Berkeley, California

**A Model System to Obtain Structural Information from the Bacterial-Mineral Interface by Neutron Reflectivity**
L Liang, A Johs, Oak Ridge National Laboratory, Oak Ridge, Tennessee

**A Nanoconfined Plasmonic Light Source for Imaging and Spectroscopy with Ultrahigh Spatial and Temporal Resolution**
MB Raschke, RL Olmon, University of Washington, Seattle, Washington

**A Periodic Density Functional Study of VOx Clusters Supported on the Defected Anatase $TiO_2$ (101) Surface**
AT Bell, V Shapovalov, University of California, Berkeley, Berkeley, California

**A Proteomic Dissection of the Hg(II) Toxicity Paradox**
SM Miller, University of California, San Francisco, San Francisco, California
AO Summers, University of Georgia, Athens, Georgia

**A Proteomic Investigation of Changes in Lipid Droplet-Bound Proteins**
SP Gross, University of California, Irvine, Irvine, California

**A Proteomic Perspective of Biodiversity**
SJ Callister, Pacific Northwest National Laboratory, Richland, Washington
JJ Parnell, ME Pfrender, Utah State University, Logan, Utah

**_Ab initio_ Studies on Voltage Gating of Ion Channels**
ME Green, VS Znamenskiy, S Liao, City College of New York, New York, New York

**Abiotic Reduction of U(VI) by Sorbed Fe(II) and the Implications for Field-Scale Bioremediation at the Rifle IFC Project Site**
R Kukkadapu, EMSL, Richland, Washington
J Davis, KM Campbell, US Geological Survey, Menlo Park, Menlo Park, California

**Absorption and Emission of Radiation in Materials**
SH Garofalini, Rutgers University, Piscataway, New Jersey
SM Kathmann, R Devanathan, RM Van Ginhoven, Pacific Northwest National Laboratory, Richland, Washington
PA Moreira, Universidade Estadual De Campinas, Sao Paulo, Brazil
JD Musgraves, LR Corrales, OA Monti, B Potter, MH De Silva, Hn Chandra, LK Schirra, BL Mooney, EA Randtke, University of Arizona, Tucson, Arizona

**Accelerated Fuel-Cladding Interaction Study using Surrogate Materials**
CH Henager, C Windisch, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, C Wang, EMSL, Richland, Washington

**Accurate _ab initio_ Determinations of Thermochemistry of Novel Molecular Radicals, Cations and Neutrals of Relevance to Combustion, Environmental, and Atmospheric Chemistry**
C Ng, C Lam, C Houchins, University of California, Davis, Davis, California
K Lau, City University of Hong Kong, Kowloon, Hong Kong, Hong Kong
S Chiu, National Center for Supercomputing Applications, Urbana, Illinois

**Accurate Embedded-Cluster Modeling of Insulators: Applications to Metal Oxide Surface Chemistry & Surface Excitation Processes**
PV Sushko, London, University College, London, United Kingdom
Z Dohnalek, AG Joly, Pacific Northwest National Laboratory, Richland, Washington
N Govind, K Kowalski, EMSL, Richland, Washington
MJ Wolf, University College London, London, United Kingdom

**Activation and Dissociation of Large Molecules in Mass Spectrometry**
J Laskin, Pacific Northwest National Laboratory, Richland, Washington
JS Smith, University of Washington, Seattle, Washington
Z Yang, University of Colorado Boulder, Boulder, Colorado

**Active Standoff Detection of Low-Volatility Chemicals on Soils Using Infrared Reflection-Absorption Spectroscopy (NNSA, PNNL Scope #25399)**
TA Blake, Pacific Northwest National Laboratory, Richland, Washington
PL Gassman, EMSL, Richland, Washington

**Addressing Challenges in Nanoscale Characterization**
DC Johnson, SL Golledge, University of Oregon, Eugene, Oregon
DJ Gaspar, A Miracle, AL Bunn, BJ Tarasevich, GE Fryxell, XS Li, RJ Orth, DW Matson, CR Yonker, K Wallace, J Teeguarden, J Liu, D wang, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington
A Gupta, Battelle Columbus, Columbus, Ohio

**Adhesion of Polymer Spheres to Modified Natural Fibers**
JD Holbery, D Howe, C Huang, Pacific Northwest National Laboratory, Richland, Washington
PL Gassman, MH Engelhard, B Arey, EMSL, Washington

**Advanced Diagnostic Studies of Lithium Ion Batteries Using In Situ and Ex Situ NMR Spectroscopies**
J Hu, L Wang, J Zhang, Z Yang, J Liu, D Choi, D Wang, Pacific Northwest National Laboratory, Richland, Washington
J Sears, EMSL, Richland, Washington

**Advanced Peta-Scale Molecular Dynamics Simulations**
TP Straatsma, J Nieplocha, BJ Palmer, EG Stephan, TA Da Silva, CL Baird, DO Apiyo, Pacific Northwest National Laboratory, Richland, Washington
MS Sansom, University of Oxford, Oxford, United Kingdom
JW Essex, University of Southampton, Southampton, United Kingdom
V Cojocaru, EML Research gGmbH, Heidelberg, Germany
MW Zacharias, Jacobs University Bremen, Bremen, Germany
RC Wade, EML Research GmbH, 69118 Heidelberg, Germany

**Advanced Proteomics and Metabolomics Studies of Type 1 Diabetes**
TO Metz, JM Jacobs, DG Camp, Pacific Northwest National Laboratory, Richland, Washington

**Advanced Proteomics and Metabolomics Studies of Type 2 Diabetes and Pre-Diabetes**
TO Metz, RD Smith, DG Camp, W Qian, Pacific Northwest National Laboratory, Richland, Washington
J Baynes, University of South Carolina, Columbia, South Carolina
R Hoffman, University of Leipzig, Leipzig, Germany

**Advances in Understanding Electron Transfer Kinetics at Environmental Interfaces**
AL Neal, University of Georgia, Aiken, South Carolina
KM Rosso, SN Kerisit, Z Wang, ES Ilton, S Yanina, TC Droubay, P Zarzycki, Pacific Northwest National Laboratory, Richland, Washington
DM Smith, Whitman College, Walla Walla, Washington
CS Lo, Washington University in St. Louis, St. Louis, Missouri
J Boily, Umea University, Umea, Sweden

**Age Related Post Translational Modifications to Proteins that Alter Protein Complexes Determined by FTICR-MS**
HS Smallwood, Pacific Northwest National Laboratory, Richland, Washington

**Airborne Measurement of Dimethylsulfide, Isoprene, and Other Trace Volatile Organic Compounds using a Proton Transfer Reaction Mass Spectrometer during the 2008 DOE ASP VOCALS Field Campaign**
Y Lee, Brookhaven National Laboratory, Upton, New York
L Alexander, EMSL, Richland, Washington

**Alpha Project Phosphoproteomics**
DG Camp, RA Maxwell, RD Smith, Pacific Northwest National Laboratory, Richland, Washington

O Resnekov, Molecular Sciences Institute, Berkeley, California

**Amorphous Semiconductor Analysis using Ion Beam Tools**
CH Henager, J Ryan, BR Johnson, Pacific Northwest National Laboratory, Richland, Washington

**An Experimental and Data Analysis Investigation into the Trapped Gases and Non-Ice Material in the Surfaces of the Outer Planets Icy Satellites and Our Moon**
CA Hibbitts, Johns Hopkins University, Laurel, Maryland
J Szanyi, Pacific Northwest National Laboratory, Richland, Washington

**An Integrated Approach to Quantifying the Coupled Biotic and Abiotic Mechanism, Rates and Long-Term Performance of Phosphate Barriers for In Situ Immobilization of Uranium**
DM Wellman, A Miracle, EM Pierce, En Richards, MA Covert, TE Queen, M Oostrom, Pacific Northwest National Laboratory, Richland, Washington
JB Nelson, Whitman College, Walla Walla, Washington
TW Wietsma, EMSL, Richland, Washington

**An NMR Study of the Complex Formed by Viral Protein vCCI and Human Chemokine Eotaxin**
W Tian, PJ LiWang, L Zhang, Texas A&M University, College Station, Texas

**Analysis of Interfacial Layers in Bimetals after Heat Treatment**
I Bae, S Hong, Pacific Northwest National Laboratory, Richland, Washington

**Analysis of Metabolic Responses to Signals from the Oncogene c-Myc a Regulator of Cell Growth and Proliferation**
NG Isern, EMSL, Richland, Washington
FM Morrish, DM Hockenbery, Fred Hutchinson Cancer Research Center, Seattle, Washington
MA Portman, Children's Hospital and Regional Medical Center, Seattle, Washington

**Analysis of Organic Oligomers Forming Secondary Aerosol from Wood Combustion-Derived Phenols**
C Anastasio, PG Green, AM Dillner, MJ Kleeman, University of California, Davis, Davis, California
J Laskin, Pacific Northwest National Laboratory, Richland, Washington
Y Dessiaterik, Colorado State University, Fort Collins, Colorado
A Laskin, EMSL, Richland, Washington

**Analysis of POSIX I/O Extensions**
RJ Latham, Argonne National Laboratory, Argonne, Illinois
EJ Felix, EMSL, Richland, Washington

**Analysis of Self-Assembled Monolayers on Mesoporous Supports (SAMMS) Materials**
JT Bays, RJ Wiacek, RS Addleman, A Cinson, J Davidson, CA Fernandez, Pacific Northwest National Laboratory, Richland, Washington

**Analysis of the Proteome and Transcriptome of *in vivo Brucella spp.*, *Yersinia pestis*, *Francisella tularensis*, *Mycobacterium spp.*, *Salmonella typhimurium* Infected Ileum**

JE Turse, Pacific Northwest National Laboratory, Richland, Washington
LG Adams, Texas A&M University, College Station, Texas

**Analysis of Zinc Environments in Singlet Oxygen-Responsive Proteins**
AS Lipton, Pacific Northwest National Laboratory, Richland, Washington
TJ Donohue, University of Wisconsin-Madison, Madison, Wisconsin

**Application of High-Throughput Proteomics**
SJ Giovannoni, Oregon State University, Corvallis, Oregon
SB Levy, Tufts University School of Medicine, Boston, Massachusetts
L Shapiro, E Toro, LC Britos, Stanford University, Stanford, California
MS Lipton, JE Turse, E Zink, BM Ham, JC Scholten, T Taverner, H Zhang, Pacific Northwest National Laboratory, Richland, Washington
TJ Donohue, University of Wisconsin-Madison, MADISON, Wisconsin
A Tsapin, University of Southern California, Los Angeles, California
T Mester, University of Massachusetts, Amherst - Biochemistry and Molecular Biology, Amherst, Maryland
DR Lovley, University of Massachusetts Amherst, Amherst, Massachusetts
S Kaplan, UT-Houston Medical School, Houston, Texas

**Assembly of the mRNA 3'-End Processing Machinery**
G Varani, TC Leeper, DW Begley, University of Washington, Seattle, Washington

**Associate Professor of Chemistry**
RL Luck, Michigan Technological University, Houghton, Michigan

**Atomically Resolved Studies of Catalytic and Photocatalytic Processes on $TiO_2$(110)**
S Li, Tulane University, New Orleans, Louisiana
Z Dohnalek, BD Kay, Z Zhang, R Rousseau, Pacific Northwest National Laboratory, Richland, Washington
JM White, University of Texas at Austin, Austin, Texas

**Automated Image Analysis of Low Frequency Radiation Induced Genomic Instability in Human Colon Carcinoma Cells**
MB Sowa, Pacific Northwest National Laboratory, Richland, Washington
GR Holtom, Harvard University, Cambridge, Massachusetts
WF Morgan, University of Maryland, Baltimore, Maryland
BL Lamarche, DF Hopkins, EMSL, Richland, Washington

**Automated Image Analysis of Low Frequency Radiation Induced Genomic Instability in Human Colon Carcinoma Cells**
MB Sowa, WJ Harvey, Pacific Northwest National Laboratory, Richland, Washington
WF Morgan, University of Maryland, Baltimore, Maryland
BL Lamarche, DF Hopkins, EMSL, Richland, Washington

**Basis of Microbial Membrane Attachment to Mineral Surfaces and Ionic Contaminants Uptake**
RD Lins, Pacific Northwest National Laboratory, Richland, Washington
M Valiev, EMSL, Richland, Washington
BH Lower, The Ohio State University, Columbus, Ohio

**Benchmark Modeling of Aerosol-Cloud Interactions**

M Ovtchinnikov, RC Easter, JM Comstock, J Fan, Pacific Northwest National Laboratory, Richland, Washington

**Benchmark Non-Born--Oppenheimer Calculations on Small Molecules**
S Bubin, L Adamowicz, University of Arizona, Tucson, Arizona

**Biasing Conformational Mobility of Unstructured Proteins by Macromolecular Crowding**
GW Daughdrill, University of Idaho, Moscow, Idaho
GW Buchko, Pacific Northwest National Laboratory, Richland, Washington

**Biogeochemistry of Oxidation-Reduction Cycling of Uranium and Iron**
WD Burgos, Pennsylvania State University, University Park, Pennsylvania

**Biocompatible, Engineered Surfaces of Mixed Chemistry**
V Hlady, University of Utah, Salt Lake City, Utah

**Biofilm Reactor Development and Characterization Studies**
H Beyenal, RS Renslow, HD Nguyen, A Bulbul, Washington State University, Pullman, Washington

**Biogeochemical Processes Responsible for the Enhanced Transport of Plutonium under Transient Unsaturated Condtions**
H Nitsche, University of California, Berkeley, Berkeley, California
R Kukkadapu, EMSL, Richland, Washington
DI Kaplan, Savannah River National Laboratory, Aiken, South Carolina

**Bioinformatics Tools to Define the Proteomic State of the Cell**
WR Cannon, GA Anderson, CS Oehmen, KH Jarman, A Heredia-Langner, DJ Taasevigen, JE Mcdermott, V Petyuk, Pacific Northwest National Laboratory, Richland, Washington
DJ Baxter, EMSL, Richland, Washington
JM Malard, SIMUCAD Design Automation, Santa Clara, California

**Biological Templates f or Synthesis of Ordered Ceramic Nanostructures**
Y Shin, G Exarhos, C Windisch, Pacific Northwest National Laboratory, Richland, Washington
B Arey, MH Engelhard, EMSL, Richland, Washington

**Biomarker Development for Chronic Obstructive Pulmonary Disease**
DL Springer, J Pounds, Pacific Northwest National Laboratory, Richland, Washington
RE Johnson, Battelle Columbus, Columbus, Ohio

**Biomarker Discovery in Pathogens by Proteomics**
MS Lipton, Pacific Northwest National Laboratory, Richland, Washington

**Biomarker Discovery Tools Development**
K Petritis, Pacific Northwest National Laboratory, Richland, Washington

**Biomarkers of Malaria Infection**
M Fried, Seattle Biomedical Research Institute, Seattle, Washington

**Biomineralology and Ultrastructure of Neutrophilic Iron-Oxidizing Bacteria**

KJ Edwards, University of Southern California, Los Angeles, California
CS Chan. Woods Hole Oceanographic Institution, Woods Hole, Massachusetts

**Biotemplated Nanoparticles for Imaging and Drug Delivery**
Y Lin, A Ma-ham, Pacific Northwest National Laboratory, Richland, Washington
Hn Liao, Xiamen University, Xiamen, Fujian, China
K Pinwattana, Chulalongkorn University, Patuwan, Bangkok, Thailand
D Du, Central China Normal University, Wuhan, Hubei, China
S Zhang, Harbin Institute of Technology, Harbin, China
Y Zhang, Hunan Normal University, Changsha, Hunan, China

**Biqing Liang's Proposal**
B Liang, JC Lehmann, Cornell University, Ithaca, New York

**Blanca Lupiani's Proposal**
BM Lupiani, SM Reddy, Texas A&M University, College Station, Texas

**Bone Growth on Tailored Biomimetic Surfaces**
MI Laitinen, S Sangyuenyongpipat, University of Jyvaskyla, Jyvaskyla, Finland
HJ Whitlow, University of Jyväskylä, University of Jyväskylä, Finland

**Bradley Tebo's Proposal**
BM Tebo, Oregon Health Sciences University/Oregon Graduate Institute, Portland, Oregon

**Breast Cancer Biomarkers in Nipple Aspirate Fluid**
RC Zangar, Pacific Northwest National Laboratory, Richland, Washington

**Burkholderia Proteomoics**
JE Turse, Pacific Northwest National Laboratory, Richland, Washington
SE Schutzer, University of Medicine and Dentistry, New Jersey Medical School, Newark, New Jersey

**Calculation of Oxygen Surface Diffusion on Bulk Oxygen Ion Conductors**
FB Prinz, TP Holme, Stanford University, Stanford, California

**Capture and Reduction of Metal Ions Out of the Environment by Biomolecular Systems**
RD Lins, TP Straatsma, B Clowers, E Baker, TA Da Silva, Pacific Northwest National Laboratory, Richland, Washington
M Valiev, WA De Jong, EMSL, Richland, Washington
J Boily, Umea University, Umea, Sweden
DA Dixon, MT Nguyen, VE Jackson, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
U Rothlisberger, M Guglielmi, EPFL Swiss Federal Institute of Technology, Lausanne, Switzerland
OV Oliveira, Federal University of Sao Carlos, Sao Carlos, Brazil
BH Lower, The Ohio State University, Columbus, Ohio

**Catalytic and Optical Properties of Surface Attached and Matrix Embedded Quantum Dots**
G Duscher, North Carolina State University, Raleigh, North Carolina

**Catalytic Studies of Transition Metal Oxide Monolayers Supported on Metal Single Crystal Surfaces**
Q Ge, Y Pan, Southern Illinois University, Carbondale, Illinois
Z Dohnalek, R Rousseau, Z Zhang, Pacific Northwest National Laboratory, Richland, Washington
F Netzer, Karl-Franzens-University Graz, Graz, Austria

**Cellular Response to Virus Infection: Global Proteome Analysis of Macaque Models of HIV and Influenza Infection**
MG Katze, DL Diamond, University of Washington, Seattle, Washington

**Ceria Nanomonitors for Trace Oxygen Monitoring in Portable Energy Systems**
S Prasad, RK Reddy, S Gupta, YS Yadav, VL Venkatraman, DB Meka, Portland State University, Portland, Oregon
MH Engelhard, EMSL, Richland, Washington
R Sanghavi, Arizona State University, Arizona

**Characterization of Amorphous Oxide Transparent Semiconductors**
GS Herman, WF Stickle, CE Otis, CM Mcconica, RL Hoffman, SD Leith, Hewlett-Packard Company, Corvallis, Oregon

**Characterization of Application-Relevant Biosilica-Precipitating Peptides of a Diatom**
G Roesijadi, JK Magnuson, Pacific Northwest National Laboratory, Richland, Washington
EV Armbrust, University of Washington, Seattle, Washington

**Characterization of Bio-Inspired Photonic Crystals for Enhancing Solar Energy Conversion by Single-Molecule Spectroscopy**
GL Rorrer, D Gale, Oregon State University, Corvallis, Oregon
D Hu, ME Jones, Pacific Northwest National Laboratory, Richland, Washington

**Characterization of Chemistry and Physics at Metal-Polythiophene and Metal-Carbon Interfaces**
LM Porter, KA Singh, PB Kulkarni, Carnegie Mellon University, Pittsburgh, Pennsylvania

**Characterization of Mercury Reduction by Fe(II) Minerals**
N Yee, Rutgers University, New Brunswick, New Jersey

**Characterization of Nanomaterials in Support of the NTP Nanotechnology Safety Initiative**
TA Cristy, Battelle Columbus, Columbus, Ohio

**Characterization of Nanostructured Catalysts and Nanostructured Materials**
J Liu, D wang, Q Huo, Pacific Northwest National Laboratory, Richland, Washington

**Characterization of Novel DNA/Semiconductor Nanoconjugates**
F Zhou, D Jiang, California State University, Los Angeles, Los Angeles, California

**Characterization of Organic Aerosols throughout the Depth of an Urban Planetary Boundary Layer: Proposed Field Deployment of EMSL Mass Spectrometers**
JP Stutz, University of California, Los Angeles, Los Angeles,, California
CM Berkowitz, R Zaveri, Pacific Northwest National Laboratory, Richland, Washington

R Zhang, Texas A&M University, College Station, Texas
D Worsnop, JT Jayne, Aerodyne Research Inc, Billerica, Massachusetts

**Characterization of Protein Confinement in Functionalized Nanoporous Supports**
C Lei, Pacific Northwest National Laboratory, Richland, Washington

**Characterization of Signaling Events Induced by Low Dose Ionizing Radiation**
DL Stenoien, Pacific Northwest National Laboratory, Richland, Washington
R Zhao, EMSL, Richland, Washington

**Characterization of Solid Oxide Fuel Cell Electrodes after Exposure**
O Marina, LR Pederson, GW Coffey, X Zhou, CD Nguyen, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington

**Characterization of Synthesized Mixed Valent Naturally Occurring Fe-Films**
GH Grathoff, Portland State University, Portland, Oregon

**Characterization of the Local Order of Organic Thin Film Material by Combined Atomic Force Microscopy and Optical Microscopy**
D Hu, AB Padmaperuma, H Qiao, PE Burrows, Pacific Northwest National Laboratory, Richland, Washington
PF Barbara, University of Texas at Austin, Austin, Texas

**Characterization of the SATB1 Phosphorylations upon Ionization Radiation**
R Zhao, EMSL, Richland, Washington
T Kohwi-Shigematsu, J Li, Lawrence Berkeley National Laboratory, Berkeley, California

**Characterizing Biofilm Development of a Bacterial Biological Control Agent**
WF Mahaffee, PK Wallace, Oregon State University, Corvallis, Oregon

**Characterizing the Composition, Morphology and Reactivity of Bacterial Nanowires using Advanced Scanning Probe Microscopy, MS-Based Proteomics and Scanning Electron Microscopy**
YA Gorby, J. Craig Venter Institute, La Jolla, California

**Characterizing the Effects of Iron- and Sulfate-Reduction on Aquifer Mineralogy: Linking Geophysics and Geomicrobiology**
JF Banfield, University of California, Berkeley, Berkeley, California
KH Williams, Lawrence Berkeley National Laboratory, Berkeley, California

**Chemical and Physical Properties of Biomass Burning Aerosol**
JL Hand, JL Collett, SM Kreidenweis, Y Dessiaterik, Colorado State University, Fort Collins, Colorado
A Laskin, C Wang, EMSL, Richland, Washington

**Chemical Kinetics and Dynamics at Interfaces: Structure and Reactivity of Ices, Amorphous Solids, and Supercooled Liquid Solutions**
J Matthiesen, RS Smith, BD Kay, Z Dohnalek, Pacific Northwest National Laboratory, Richland, Washington
T Zubkov, Ball State University, Muncie, Indiana

**Chemistry and Microphysics of Small Particles**
A Zelenyuk, J Yang, Pacific Northwest National Laboratory, Richland, Washington
K Mueller, E Nam, State University of New York at Stony Brook, Stony Brook, New York

**Chemistry of Aerosols in Mexico City: MILAGRO 2006 Study**
A Tivanski, University of Iowa, Iowa City, Iowa
KS Johnson, LT Molina, Massachusetts Institute of Technology, Cambridge, Massachusetts
Y Dessiaterik, Colorado State University, Fort Collins, Colorado
V Shutthanandan, C Wang, Z Zhu, A Laskin, TW Wietsma, EMSL, Richland, Washington
MK Gilles, RJ Hopkins, RC Moffet, Lawrence Berkeley National Laboratory, Berkeley, California

**Chemistry of Outer Solar System Materials**
TB McCord, GB Hansen, University of Washington, Seattle, Washington

**Chlorinated Methane Hydrolysis Rates**
JE Amonette, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**Chromium Diffusion Kinetics in Nano-Ceria and Doped Ceria Coatings: An UCF-PNNL Collaboration**
S Seal, RK Thanneeru, SA Deshpande, AS Karakoti, University of Central Florida, Orlando, Florida
S Kuchibhatla, EMSL, Richland, Washington

**Cluster Model Studies of Condensed Phase Phenomena**
X Wang, X Xing, Washington State University, Richland, Washington
C Chi, Fudan University, Shanghai, China
K Matheis, Universitaet Karlsruhe, Karlsruhe, Germany
L Wang, Washington State University Tri-Cities, Richland, Washington
G Xiao, Xi'an Jiaotong University, Xi'an, Shaanxi, China

**Clusters of Damage in Irradiated DNA**
MD Sevilla, D Becker, Oakland University, Rochester, Michigan
JD Zimbrick, Colorado State University, Fort Collins, Colorado
MK Bowman, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**ClusterSculptor: An Expert Driven Visual Analytics Tool for the Classification of Single Particle Mass Spectra**
A Zelenyuk, J Yang, Pacific Northwest National Laboratory, Richland, Washington
K Mueller, E Nam, State University of New York at Stony Brook, Stony Brook, New York

**Collaborative Research Projects Supported by the NCRR P41 Resource Center**
SS Rossie, Purdue University, West Lafayette, Indiana
DG Moerman, University of British Columbia, Vancouver, British Columbia, Canada
D Smith, University of California, Los Angeles, Los Angeles, California
M Pallavicini, University of California, Merced, Merced, California
S Warren, Massachusetts General Hospital East and Harvard University School of Medicine, Charlestown, Massachusetts
MM Sarwal, Stanford University, Stanford, California

DG Camp, RD Smith, W Qian, JM Jacobs, T Liu, F Yang, V Petyuk, BD Thrall, DL Stenoien, TC Squier, N Colton, BO Petritis, S Chowdhury, AT Wright, I Marginean, Pacific Northwest National Laboratory, Richland, Washington
N Sonenberg, McGill University, Montreal, Quebec, Canada
L Pasa-Tolic, R Zhao, HM Mottaz, EMSL, Richland, Washington
MG Katze, J Cuschieri, University of Washington, Seattle, Washington
M Ginsberg, RL Klemke, University of California, San Diego, La Jolla, California
JS Kim, Seoul National University, Seoul, Korea South, Republic Of
J Nelson, Oregon Health Sciences University/Oregon Graduate Institute, Portland, Oregon
T Kohwi-Shigematsu, Lawrence Berkeley National Laboratory, Berkeley, California
A Umar, Erasmus University Medical Center, Rotterdam, Rotterdam, Netherlands
JA Mannick, JA Lederer, Harvard Medical School, Boston, Massachusetts
RN Kulkarni, Joslin Diabetes Center, Boston, Massachusetts

**Combinatorial Operando Catalyst Research**
D Hu, ZC Zhang, G Xia, C Windisch, Pacific Northwest National Laboratory, Richland, Washington

**Combinatorial Operando Catalyst Research**
D Hu, ZC Zhang, G Xia, G Li, Pacific Northwest National Laboratory, Richland, Washington

**Combined NMR/Optical Microscopy of Biofilm Physiology Studies**
R Lux, University of California, Los Angeles, Los Angeles, California
PD Majors, J McLean, Pacific Northwest National Laboratory, Richland, Washington

**Combining *in-situ* Buffer-Layer-Assisted-Growth with Scanning Probe Microscopy for Formation and Study of Supported Model Catalysts**
I Lyubinetsky, Environmental Molecular Sciences Laboratory, Richland, Washington

**Community-Based Biosignatures of Exposure and Functional Response in the Sediment-Water Interface of the Hyporheic Zone and Periphyton Community in River Systems**
J Small, AL Bunn, Pacific Northwest National Laboratory, Richland, Washington

**Community Proteomic Analysis of a Near-Shore Anoxic Basin: Saanich Inlet**
SJ Hallam, University of British Columbia, Vancouver, British Columbia, Canada
AD Norbeck, Pacific Northwest National Laboratory, Richland, Washington

**Comparative Proteomic Analysis of Naturally Occurring Anaerobic Methane Oxidizing Communities**
SJ Hallam, University of British Columbia, Vancouver, British Columbia, Canada
AD Norbeck, Pacific Northwest National Laboratory, Richland, Washington

**Complex Enzymatic Reactions**
TP Straatsma, TA Da Silva, DO Apiyo, Pacific Northwest National Laboratory, Richland, Washington
H Michel, E Herzog, Max Planck Institute of Biophysics, Frankfurt am Main, Germany
VH Helms, W Gu, Universitat des Saarlandes, Saarbrucken, Germany
DE Gomes, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil
M Elstner, Technical University Braunschweig, Braunschweig, Germany

**Composition Analysis of Surface-Bound Nanoparticle Monolayers**
ML Jespersen, JE Hutchison, JA Dahl, University of Oregon, Eugene, Oregon

**Compositionally Graded V2O5 for Improved Thermoelectric Power**
A Yamamoto, AIST, Ibaraki, Japan
F Ohuchi, S Iwanaga, University of Washington, Seattle, Washington

**Computational and Experimental Investigations on NMR Properties of Actinide Compounds**
J Li, HM Cho, SD Burton, Pacific Northwest National Laboratory, Richland, Washington

**Computational Chemical Dynamics of Complex Systems**
SL Mielke, Northwestern University, Evanston, Illinois
J Gao, CJ Cramer, DG Truhlar, JI Siepmann, DM York, EE Dahlke, P Jaque, ZH Li, R Valero Montero, A Sorkin, O Tishchenko, Y Zhao, JD Scanlon, K Wong, W Xie, Y Zhou, A Cembran, S Ma, JL Rafferty, K Nam, AN Jay, BJ Lynch, KE Anderson, EA Amin, J Zheng, BA Ellingson, Y Fan, A Marenich, RM Olson, HR Leverentz, University of Minnesota, Minneapolis, Minnesota
SM Kathmann, M Dupuis, GK Schenter, B Ginovska, V Glezakou, CJ Mundy, P Fan, Pacific Northwest National Laboratory, Richland, Washington
MB Tsai, Brookhaven National Laboratory, Upton, New York
A Heyden, University of South Carolina, Columbia, South Carolina
M Valiev, K Kowalski, EMSL, Richland, Washington
MA Iron, Weizmann Institute, Rehovot, Israel
A Chakraborty, Pennsylvania State University, University Park, Pennsylvania

**Computational Design of Catalysts: The Control of Chemical Transformation to Minimize the Environmental Impact of Chemical Processes**
JM Caruthers, KA Novstrup, JM Switzer, Purdue University, West Lafayette, Indiana
MA Barteau, AC Lukaski, University of Delaware, Newark, Delaware
Q Ge, L Cheng, Southern Illinois University, Carbondale, Illinois
A Altun, I Kerkines-Keramidas, AE Kuznetsov, Emory University, Atlanta, Georgia
K Morokuma, Kyoto University, Kyoto, Japan
RL Abel, Columbia University, New York, New York
D Camaioni, J Li, Dn Mei, J Franz, M Dupuis, NA Deskins, R Rousseau, Pacific Northwest National Laboratory, Richland, Washington
F Mehmood, Argonne National Laboratory, Argonne, Illinois
WF Schneider, RB Getman, University of Notre Dame, Notre Dame, Indiana
CR Landis, E Mavrikakis, LC Grabow, PA Ferrin, RP Nabar, AU Nilekar, FM Eichhorn, G Peng, University of Wisconsin-Madison, Madison, Wisconsin
JF Haw, DM McCann, University of Southern California, Los Angeles, California
M Neurock, VM Vadhri, C Buda, CP Plaisance, Y Cai, University of Virginia, Charlottesville, Virginia
DA Dixon, S Li, M Hernandez Matus, MT Nguyen, DJ Grant, R Craciun, T Wang, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
L Xu, University of Texas at Austin, Austin, Texas
J Du, University of North Texas, Denton, Texas
MJ Janik, Pennsylvania State University, University Park, Pennsylvania
MS Gutowski, S Ling, Heriot-Watt University, Edinburgh, United Kingdom
DC Ford, J Jiao, JA Herron, CA Farberow, University of Wisconsin, Madison, Madison, Wisconsin
L Wang, Washington State University Tri-Cities, Richland, Washington

**Computational Design of Materials for Hydrogen Storage**
P Jena, Qn Wang, Q Sun, S Li, K Boggavarapu, Virginia Commonwealth U, Richmond, Virginia
CE Strickland, Washington State University, Pullman, Washington
Z Zhang, Stanford University, Stanford, California
J Li, JE Jaffe, SM Kathmann, GK Schenter, CJ Mundy, Pacific Northwest National Laboratory, Richland, Washington
A Nikitin, Stanford Linear Accelerator Center, Menlo Park, California
PJ Hay, N Henson, Los Alamos National Laboratory, Los Alamos, New Mexico
W Stier, L Arnadottir, A Arnaldsson, K Tsemekhman, University of Washington, Seattle, Washington
DA Dixon, DJ Grant, JR Batson, Mn Hernandez Matus, MT Nguyen, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
GA Henkelman, University of Texas at Austin, Austin, Texas
H Jonsson, University of Iceland, Reykjavík, Iceland
RA Bachorz, Universitaet Karlsruhe, Karlsruhe, Germany
MS Gutowski, A Whiteside, RG McKinlay, AV Abramov, Heriot-Watt University, Edinburgh, Russian Federation

**Computational Investigation of Metal Clusters on Doped Carbon Supports**
CH Turner, CK Acharya, W An, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**Computational Rheology of Dense Suspensions**
A Chatterjee, DR Heine, Corning, Inc., Corning, New York

**Computational Studies of the Heterogeneous Production of Molecular Chlorine by OH Oxidation of Chloride in Sea Salt**
DJ Tobias, R D'auria, University of California, Irvine, Irvine, California
SS Xantheas., Pacific Northwest National Laboratory, Richland, Washington

**Computational Study of Chiral Separations by Ion Mobility Spectrometry**
AE Clark, NL Zakharova, Washington State University, Pulman, Washington

**Computational Study of Protein-Protein Interaction Dynamics at Single Molecule Level**
JN Wang, Q Lu, State University of New York at Stony Brook, Stony Brook, New York
HP Lu, Bowling Green State University, Bowling Green, Ohio

**Computer Simulation of Defects and Interfaces in Nuclear Fuel Materials**
R Devanathan, J Yu, K Artiga, S Morrison-Smith, EE Moore, Pacific Northwest National Laboratory, Richland, Washington
PA Moreira, Universidade Estadual De Campinas, Sao Paulo, Brazil

**Conceptual Animations of Efficient Enzymes within Functionalized Mesoporous Silica**
MC Perkins, EJ Ackerman, KR Swanson, Pacific Northwest National Laboratory, Richland, Washington

**Conformational Dynamics of Pin1 Regulation of APP Processing and Abeta Production**
LK Nicholson, Cornell University, Ithaca, New York

**Contribution of Biosorption Processes to the Sustained Removal of Uranium from Groundwater in the Absence of Added Electron Donor**
LA N'guessan, DR Lovley, University of Massachusetts Amherst, Amherst, Massachusetts

**Coprecipitation of Aluminum Hydroxides and Calcium Carbonates during Denitrification: A Stabilization Strategy for Oxidized Metals and Radionuclides**
JD Istok, Oregon State University, Corvallis, Oregon
M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**Correlating the Active Site Structure of Copper Metalloproteins with their Spectroscopic and Chemical Properties**
AS Lipton, Pacific Northwest National Laboratory, Richland, Washington
GS Harbison, University of Nebraska, Lincoln, Nebraska

**Correlation of Structure and Function of Zinc Metalloproteins Via a Combined NMR/Molecular Theory Approach**
G Parkin, Columbia University, New York, New York
AS Lipton, PD Ellis, R Heck, TP Straatsma, Pacific Northwest National Laboratory, Richland, Washington
CA Fierke, M Hernick, J Penner-Hahn, University of Michigan, Ann Arbor, Michigan
M Valiev, EMSL, Richland, Washington

**Coupled Hydrological and Geochemical Studies on Uranium Plumes at Hanford Site: Reactions, Spatial Distributions, Speciation, and Future Mobility**
Z Wang, Pacific Northwest National Laboratory, Richland, Washington

**Coupling Temporal Variations in Geochemistry to Activities of Microbial Populations in the Deep Sub-Sea-Floor Biosphere**
JE Turse, Pacific Northwest National Laboratory, Richland, Washington
PR Girguis, JC Robidart, Harvard University, Cambridge, Massachusetts

**Course in Nanoscience and Nanotechnology**
S Gupta, Portland State University, Portland, Oregon
RD Souza, Y Qiang, C Berven, DS Choi, University of Idaho, Moscow, Idaho
A Datta, GC Eastland, X Ye, L Zhang, AR Smith, Washington State University, Pullman, Washington
N Karri, Pacific Northwest National Laboratory, Richland, Washington
DR Baer, EMSL, Richland, Washington
F Ohuchi, University of Washington, Seattle, Washington
MV Peeler, Washington State Department of Ecology, Olympia, Washington
L Wang, Washington State University Tri-Cities, Richland, Washington

**Cryo-EM Investigations of Interfacial Bacterial Extracellular Polymeric Substance (EPS) in Vanadium Interactions**
MJ Marshall, Pacific Northwest National Laboratory, Richland, Washington

**Cryogenic XPS Study of Metal Oxide/Water Interfaces**
J Boily, Umea University, Umea, Sweden

**Cryo-TEM Investigation of Polyketide Synthase Megacomplexes in *Candidatus Endobugula sertula* and *Teredinibacter turnerae***
A Dohnalkova, EMSL, Richland, Washington
MG Haygood, AE Silva, Oregon Health Sciences University/Oregon Graduate Institute, Beaverton, Oregon

**Cyanobacteria Membrane Biology Grand Challenge: Systems Analysis of the Dynamics of Membrane Architecture, Composition, and Function- Proteomic, Metabolomic, and Metallomic Characterization**
JM Jacobs, DW Koppenaal, TO Metz, Q Zhang, Pacific Northwest National Laboratory, Richland, Washington
HB Pakrasi, J Stockel, Washington University in St. Louis, St. Louis, Missouri

**Data Assimilation, Visualization, and Mining**
ES Peterson, Pacific Northwest National Laboratory, Richland, Washington

**Deep Desulphurization of Hot Coal Gas for Production of Liquid Fuels**
L Li, J Male, R Vedula, Pacific Northwest National Laboratory, Richland, Washington

**Defects and Defect Processes in Ceramics**
WJ Weber, W Jiang, I Bae, BD Milbrath, Pacific Northwest National Laboratory, Richland, Washington
L Boatner, Oak Ridge National Laboratory, Oak Ridge, Tennessee
X Xiang, University of Michigan, Ann Arbor, Michigan
R Linares, Universidade de Sao Paulo, Sao Paulo, Brazil
Y Zhang, EMSL, Richland, Washington

**Degradation of Lignin Using Homogeneous Catalysis in Ionic Liquids**
G Li, SD Burton, ZC Zhang, AS Lea, JE Amonette, Pacific Northwest National Laboratory, Richland, Washington
JM White, University of Texas at Austin, Austin, Texas

**Demonstrate a Systematic Application of a Magnetic Tweezers: Holding a Protein Molecule in Solution**
HP Lu, Bowling Green State University, Bowling Green, Ohio

**Dependence of High Affinity of Metalloprotease for Inhibitor on Internal Millisecond Motions**
SR Van Doren, University of Missouri, Columbia, Columbia, Missouri

**Design Criteria for Organic Charge Transporting Materials through Computational Modeling**
L Sapochak, AB Padmaperuma, PE Burrows, Pacific Northwest National Laboratory, Richland, Washington
M Valiev, N Govind, EMSL, Richland, Washington

**Desiccation of Porous Media to Limit Contaminant Migration**
M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
JH Dane, Auburn University, Auburn, Alabama
TW Wietsma, EMSL, Richland, Washington

**Design of Micro-Cantilever Actuators for Measuring Surface Tension of Sub Microliter Volumes Applied Towards Monitoring Interfacial Processes**
DW Britt, BA Henrie, Utah State University, Logan, Utah

**Detailed Characterization of Arsenic Adsorptive Media**
MH Engelhard, EMSL, Richland, Washington
DT Kremser, BM Sass, Battelle Columbus, Columbus, Ohio

**Detection of Gas Inclusion in Organic and Metal-Organic Solids**
P Thallapally, Pacific Northwest National Laboratory, Richland, Washington

**Determination Li Concentration in Wide Band Gap $SnO_2$ Semiconductor, Using RBS Technique**
SB Rananavare, A Chaparadza, Portland State University, Portland, Oregon

**Determination of Cr and O Diffusion Coefficients in $(Co,Mn)_3O_4$ Coatings for IT-SOFC Steel Interconnects**
RJ Smith, Montana State University, Bozeman, Montana
B Arey, C Wang, EMSL, Richland, Washington

**Determination of Enhanced ZnO Nucleation and Growth by Modeling, Simulation and MOCVD under UV Irradiation**
VT Woods, B Luttrell, G Huebner, Peak Materials, Colorado Springs, Colorado

**Determination of Saturation-Capillary Pressure Relations of Crude Oil-Brine Systems to Estimate Oil-Water Interfacial Areas**
L Zhong, Pacific Northwest National Laboratory, Richland, Washington

**Determination of the CCR5 and CXCR4 Antagonist and Agonist Binding Site**
TE Angel, EA Dratz, Montana State University, Bozeman, Montana

**Determining Mechanisms of Nonlinear Photo Response and Transport Properties in Scintillating Materials**
F Gao, TC Droubay, TC Kaspar, Pacific Northwest National Laboratory, Richland, Washington
Y Zhang, V Shutthanandan, L Saraf, EMSL, Richland, Washington
W Zhang, Peking University, Beijing, China

**Determining the Effects of Organic Chemical Mixtures and Wastewater on DNAPL Migration**
H Yoon, AJ Valocchi, C Werth, University of Illinois, Urbana, Illinois
M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**Develop Fundamental Surface Science Characterization Data for Use in Improving Mixed Alcohol Synthesis Catalysts**
JF White, SM Kathmann, D Mei, R Rousseau, Pacific Northwest National Laboratory, Richland, Washington

**Developing a Systems Biology Approach for the Termite Gut Microbial Isolate *Verrucomicrobium* sp. strain TAV2**
JL Rodrigues, University of Texas at Arlington, Arlington, Texas

**Developing an *in situ* Assay for Determining Spatial and Temporal Autoinducer Concentrations in Wound Biofilms**
KP Rumbaugh, Texas Tech University, Lubbock, Texas

**Developing Calculation Methods to Precisely Measure Proteome Proteins and Their Post-Translational Modifications**
SO Purvine, Y Shen, Pacific Northwest National Laboratory, Richland, Washington
N Tolic, KK Hixson, EMSL, Richland, Washington

**Development and Application of Advanced Tools for Computational Fluid Dynamics**
DR Rector, ML Stewart, Pacific Northwest National Laboratory, Richland, Washington

**Development of 1st Principles Dynamics with Exact Exchange and Spin-Orbit ZORA**
EJ Bylaska, Pacific Northwest National Laboratory, Richland, Washington
M Valiev, WA De Jong, EMSL, Richland, Washington
JH Weare, SA Bogatko, University of California, San Diego, La Jolla, California

**Development of a Microfluidics Flow and Transport Laboratory**
C Werth, C Zhang, University of Illinois, Urbana, Illinois
M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**Development of a Scalable Solution-based Catalyst Fabrication Process using Microreaction Technology**
C Chang, S Han, Oregon State University, Corvallis, Oregon

**Development of Alternative and Durable High Performance Cathode Supports for PEM Fuel Cells**
P Kumar, Washington State University, Pullman, Washington
Y Wang, J Liu, J Kwak, Z Zhang, VV Viswanathan, Y Shao, R Kou, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington

**Development of an Integrated Atomic Force / Fluorescence Microscope at EMSL**
Z Wang, Pacific Northwest National Laboratory, Richland, Washington
BH Lower, The Ohio State University, Columbus, Ohio

**Development of High Throughput Proteomic Production Operations (PNNL Scope # 40601, Dick Smith's OBER Proteomics)**
N Colton, RD Smith, EW Robinson, E Baker, EA Livesay, YM Ibrahim, H Kang, NM Lourette, JS Page, AK Shukla, Pacific Northwest National Laboratory, Richland, Washington
L Pasa-Tolic, EMSL, Richland, Washington
Q Luo, Northeastern University, Boston, Maine

**Development of Microscopically-Based Models for Prediction of the Impact of Surface Grain Coating on Mineral Dissolution and Leaching Rates**
KM Rosso, ES Ilton, O Qafoku, Pacific Northwest National Laboratory, Richland, Washington
AR Felmy, EMSL, Richland, Washington

J Boily, Umea University, Umea, Sweden

**Development of Novel Electrolyte and Electrode Materials for a New Generation of Low-Temperature SOFCs Using First-Principles Atomistic Thermodynamics**
M Liu, Y Choi, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia

**Development of Room Temperature Ferromagnetism in Wide-band-gap Oxide Semiconductor Nanostructures**
A Punnoose, AP Thurber, Boise State University, Boise, Idaho

**Development of Single Molecule Force Microscopy Capability to Examine the Molecular Mechanism of Lignocellulosic Material Degradation**
Z Dai, KM Rosso, Z Wang, G Orr, Pacific Northwest National Laboratory, Richland, Washington
BH Lower, The Ohio State University, Columbus, Ohio

**Development of the Novel Hybrid Nanowire-based Solar Cell on a Flexible Substrate**
DS Choi, University of Idaho, Moscow, Idaho

**Development of Time-Dependent Quantum Reaction Dynamics for Surface Reactions**
JR Rustad, University of California, Davis, Davis, California
EJ Bylaska, GK Schenter, Pacific Northwest National Laboratory, Richland, Washington
D Wang, N Govind, EMSL, Richland, Washington

**Development of Tunable Highly Efficient THz Sources using Focused Ion Beam (FIB)-Based Lithography**
SK Sundaram, BJ Riley, JV Crum, Pacific Northwest National Laboratory, Richland, Washington
L Saraf, EMSL, Richland, Washington

**Development of Tunable THz Sources using Focused Ion Beam (FIB)-Based Lithography**
SK Sundaram, P Keller, H Qiao, Pacific Northwest National Laboratory, Richland, Washington
L Saraf, EMSL, Richland, Washington

**Diffusion Measurements in Polymers and Their Composites**
LV Smith, Washington State University, Pullman, Washington

**Directed Self-Assembly of Metal Oxide Island Nanostructures**
JF Groves, University of Virginia, Charlottesville, Virginia
Y Du, DR Baer, EMSL, Richland, Washington

**Discovery of Biomarkers Related to COPD**
SM Varnum, J Pounds, Pacific Northwest National Laboratory, Richland, Washington

**Distance-Dependent Electron Transfer to Mineral Surfaces Mediated by Bacterial Multiheme Cytochromes**
NS Wigginton, MF Hochella, Virginia Polytechnic Institute, Blacksburg, Virginia
KM Rosso, Pacific Northwest National Laboratory, Richland, Washington

**DNA Methylation-Dependent Patterns of Histone Post-Translational Modification**
CS Pikaard, Washington University in St. Louis, Saint Louis, Missouri

**DNAPL-Water Interfacial Area Determinations During Entrapped DNAPL Dissolution Using Tracer Techniques**
S Bottero, Utrecht University, Utrecht, Italy
M Schroth, Swiss Federal Institute of Technology, Zurich, Switzerland

**Doping Inorganic Wide-Bandgap Semiconductors for Future Energy Devices**
W Jiang, Pacific Northwest National Laboratory, Richland, Washington

**Dynamic Changes in Molecular Interactions along the Circadian Rhythm (Orr-LDRD Membrane Biology GC, PNNL Scope #90001)**
G Orr, DJ Panther, KJ Cassens, Pacific Northwest National Laboratory, Richland, Washington
HB Pakrasi, Washington University in St. Louis, St. Louis, Missouri
T Ogawa, Shanghai Institute of Plant Physiology and Ecology, Shanghai, China

**Dynamic Characterization of the Enzyme Phosphomannomutase/Phosphoglucomutase from *P. aeruginosa***
SR Van Doren, LJ Beamer, University of Missouri, Columbia, Columbia, Missouri

**Early Transition Metal Oxides as Catalysts: Crossing Scales from Clusters to Single Crystals to Functioning Materials**
E Iglesia, University of California, Berkeley, Berkeley, California
CH Peden, J Hu, J Kwak, J Liu, Y Wang, X She, G Xia, D Kim, JF White, VM Lebarbier, L Zhang, Pacific Northwest National Laboratory, Richland, Washington
B Xu, Y Wu, Tsinghua University, Beijing, China
MH Engelhard, EMSL, Richland, Washington
DA Dixon. University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
S Cho, Chonnam National University, Guangju, Korea South, Republic Of
K Lee, Korea University, Seoul, Korea South, Republic Of

**Edgar Buck's Proposal**
EC Buck, RN Wittman, Pacific Northwest National Laboratory, Richland, Washington

**Effect of Changing Rainfall and Temperature on Biochemical Composition of Soil Organic Matter**
JF Banfield, University of California, Berkeley, Berkeley, California
AA Berhe, University of California, Merced, Merced, California
MP Waldrop, US Geological Survey, Menlo Park, Menlo Park, California

**Effect of Structure and Impurities on Charge Transfer Reactions in Solid State Electrochemical Devices**
LR Pederson, Pacific Northwest National Laboratory, Richland, Washington
S Gopalan, UB Pal, SN Basu, L Miara, KF Ludwig, KE Smith, Boston University, Boston, Massachusetts

**Effects of Nitrogen Additions on Soil Carbon Pools in Two Humid Tropical Forest Types**
DF Cusack, University of California, Berkeley, Berkeley, California

MS Torn, Lawrence Berkeley National Laboratory, Berkeley, California

**Electrochemical Analyses of the Electron Transfer Rates of MtrC and OmcA to Hematite**
L Shi, Pacific Northwest National Laboratory, Richland, Washington

**Electron Donor Dependence of the Extent and Forms of Microbially Reducible Uranium from Contaminated Sediments**
AS Madden, AV Palumbo, LA Fagan, TJ Phelps, Oak Ridge National Laboratory, Oak Ridge, Tennessee

**Electron Energy Loss in Radiation Detection Materials**
B Cannon, AJ Carman, Pacific Northwest National Laboratory, Richland, Washington
P Nachimuthu, C Wang, EMSL, Richland, Washington

**Electron Microscopy Imaging of Cyanobacteria *Synechcystis sp***
C Gassman, Columbia Basin College, Pasco, Washington
A Dohnalkova, B Arey, EMSL, Richland, Washington

**Elucidating the Structure of Surface Species on Heterogeneous Catalysts**
DA Ruddy, CA Bradley, NS Bell, TD Tilley, Lawrence Berkeley National Laboratory, University of California, Berkeley, Berkeley, California

**Enabling PVFS2 Support over Quadrics for MPP2 Cluster**
W Yu, Oak Ridge National Laboratory, Oak Ridge, Tennessee

**Enabling Quantitatively Predictive Understanding of Multifluid Flow and Multicomponent Biogeochemical Reactive Transport in Complex, Subsurface Systems**
AJ Valocchi, University of Illinois, Urbana-Champaign, Illinois
S Yabusaki, DH Bacon, VL Freedman, AM Tartakovsky, ML Rockhold, Y Fang, M Oostrom, F Zhang, AL Ward, Pacific Northwest National Laboratory, Richland, Washington
PC Lichtner, Los Alamos National Laboratory, Los Alamos, New Mexico
JC Parker, F Zhang, Oak Ridge National Laboratory, Oak Ridge, Tennessee
M White, Mississippi State University, Mississippi State, Mississippi
M Rosing, Self-Employed (Rosing), Ft. Collins, Colorado
RJ Versteeg, Idaho National Laboratory, Idaho Falls, Idaho

**Energetics, Dynamics and Mechanisms of Dissociation of Peptide Radical Cations**
IK Chu, N Lam, The University of Hong Kong, Pokfulam, Hong Kong
C Siu, York University, Toronto, Ontario, Canada
Z Yang, University of Colorado Boulder, Boulder, Colorado

**Energy and Entropy Effects in Dissociation of Non-Covalent Complexes: A Combined Experimental and Theoretical Investigation**
J Laskin, Pacific Northwest National Laboratory, Richland, Washington
Z Yang, University of Colorado Boulder, Boulder, Colorado
X Shi, JH Parks, Rowland Institute at Harvard, Cambridge, Massachusetts

**Energy Smart Data Center**
A Adhikari, Portland State University, Portland, Oregon

A Marquez, Pacific Northwest National Laboratory, Richland, Washington

**Enhanced Ionic Conductivity of Samaria Doped Ceria Thin Films through Tailoring the Dopant Concentration and Microstructures**
Z Yu, Nanjing Normal University, Nanjing, China

**Environmental Proteomic Analysis of Anaerobic Methane Oxidizing Systems**
L Constan, SJ Hallam, University of British Columbia, Vancouver, British Columbia, Canada

**Epitaxial Growth and Properties of Magnetically Doped ZnO Prepared by Pulsed Laser Deposition of Nanoparticle Targets**
MJ Hopkins, Portland State University, Portland, Oregon
DR Dixon, Washington State University, Pullman, Washington
SA Chambers, TC Droubay, TC Kaspar, Pacific Northwest National Laboratory, Richland, Washington
C Wang, EMSL, Richland, Washington
KM Whitaker, CR Johnson, KR Kittilstved, DR Gamelin, SA Santangelo, PI Archer, Y Li, ST Ochsenbein, University of Washington, Seattle, Washington

**Equilibrium-Induced Decomposition of Nitrates on a $N_{ox}$ Storage/Reduction Catalyst**
WS Epling, University of Waterloo, Waterloo, Ontario, Canada

**Evaluate and Apply the LC/FAIMS/IMS/TOF MS Platform to High Throughput Quantitative Analysis**
K Tang, E Baker, R Mabrouki, Pacific Northwest National Laboratory, Richland, Washington

**Evaluation of Newly Developed Multiuse Affinity Probes for Subdiffraction Imaging**
D Hu, TC Squier, MU Mayer-Cumblidge, Y Xiong, Pacific Northwest National Laboratory, Richland, Washington

**Excited States of DNA Hairpins**
GC Schatz, S Tonzani, Northwestern University, Evanston, Illinois

**Experimental and Theoretical Investigations on the Chemistry and Dynamics of Ammonia Borane Dehydrogenation**
MR Hartman, Oregon State University, Corvallis, Oregon
D Neiner, University of California, Davis, Davis, California
TJ Johnson, T Autrey, NJ Hess, WJ Shaw, A Karkamkar, J Li, J Linehan, CJ Mundy, SM Kathmann, D Camaioni, RG Potter, AT Luedtke, Pacific Northwest National Laboratory, Richland, Washington
CW Hamilton, H Kim, TE Proffen, Los Alamos National Laboratory, Los Alamos, New Mexico
MO Jones, University of Oxford, Oxford, United Kingdom
LR Alden, DW Himmelberger, University of Pennsylvania, Philadelphia, Pennsylvania
Y Chua, National University of Singapore, Singapore, Singapore
MH Engelhard, EMSL, Richland, Washington
ME Bowden, Industrial Research Ltd., Lower Hutt, New Zealand
WI David, Rutherford Appleton Laboratory, Chilton, Oxfordshire, United Kingdom

**Experimental and Theoretical Studies of Reaction Pathways for the Breakdown of Chlorinated Hydrocarbon Molecules by Metal and Metal Oxide Nanoparticles (including PNNL Scope # 42184/44076, Baer/Amonette/Tratnyek Nano-Fe BES/EMSP project)**
J Antony, Y Qiang, A Sharma, University of Idaho, Moscow, Idaho
RL Penn, C Chun, University of Minnesota, Minneapolis, New Mexico
M Dupuis, BD Kay, EJ Bylaska, JE Amonette, Z Dohnalek, GS Parkinson, DW Matson, Pacific Northwest National Laboratory, Richland, Washington
AA El-Azab, Florida State University, Tallahassee, Florida
R Kukkadapu, DR Baer, MH Engelhard, TW Wietsma, C Wang, S Kuchibhatla, PL Gassman, EMSL, Richland, Washington
PG Tratnyek, J Nurmi, V Sarathy, P Lee, Oregon Health Sciences University/Oregon Graduate Institute, Beaverton, Oregon
S Suzer, Bilkent University, Ankara, Turkey

**Experimental Investigation and Theoretical Validation of Growth, Morphology, and Chemistry of Cuprous Oxide Nanoclusters on STO (100) Substrate**
CH Henager, SK Sundaram, Pacific Northwest National Laboratory, Richland, Washington
S Kuchibhatla, T Thevuthasan, EMSL, Richland, Washington

**Experimental Investigation of Sr-90 Subsurface Contamination Sequestration in Hanford 100N Area Sediments by Surface Infiltration of an Apatite Solution**
JE Szecsody, M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**Experimental Investigation of Strontium Mass Transfer in a Dynamic Vadose Zone - Aquifer - River System**
EJ Bylaska, S Yabusaki, M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**Experimental Studies of Fundamental Molecule-Particle Interactions and Reactions on Iron Metal and Oxide Surfaces**
RS Smith, BD Kay, Z Dohnalek, GS Parkinson, Pacific Northwest National Laboratory, Richland, Washington

**Experimental Validation of Multiscale Modeling Approach to Materials Discovery for Radiation Detection Materials**
CH Henager, SK Sundaram, F Gao, Pacific Northwest National Laboratory, Richland, Washington
S Kuchibhatla, EMSL, Richland, Washington
Z Yu, Nanjing Normal University, Nanjing, China
Y Li, Pennsylvania State University, State College, Pennsylvania

**Exploration of the Cell Parameter and Thermal Expansion Behavior in Au and $ZrW_2O_8$ Nanoparticles**
W Douglas, J Kellar, South Dakota School of Mines and Technology, Rapid City, South Dakota

**Exploring the Mechanisms and Kinetics of Small Peptides towards the Search for the Global Minimum through Molecular Dynamics Simulations**

D Shemesh, EW Schlag, Technical University Munich, Garching, Germany

**Exploring the Proteome of *E. coli* Following Adaptation to Environmental and Genetic Perturbation**
JE Turse, Pacific Northwest National Laboratory, Richland, Washington
BO Palsson, University of California, San Diego, La Jolla, California

**Fabrication and Characterization of High-Performance Transparent Transistor**
F Hua, Clarkson University, Potsdam, New York

**Fabrication of a Carbon Nanotube Thermionic Cathode**
KJ Bunch, H Qiao, Pacific Northwest National Laboratory, Richland, Washington
PL Gassman, EMSL, Richland, Washington

**Facility-Wide Management and Storage for Scientific Data**
KJ Auberry, EMSL, Richland, Washington

**Fate and Transport of Titanium Dioxide through Freshwater Ecosystems**
DJ Gaspar, A Miracle, AL Bunn, JA Ward, Pacific Northwest National Laboratory, Richland, Washington

**Ferromagnetic Study of ZnO Based Heterojunctions**
N Athavan, R Könenkamp, Portland State University, Portland, Oregon

**FIB/SEM/EBSD/EDS Study of the Grain boundary Character Effect on Precipitation**
Y Yang, Pacific Northwest National Laboratory, Richland, Washington
L Tan, AG Certain, TR Allen, University of Wisconsin-Madison, Madison, Wisconsin

**Fine-Tuning Ambipolar Charge-Transport Properties of Organic Materials By Computational Design**
AB Padmaperuma, LS Sapochak, Pacific Northwest National Laboratory, Richland, Washington
N Govind, M Valiev, EMSL, Richland, Washington

**First Principles Adaptive Kinetic Monte Carlo Calculations of Catalytic Reactions at Supported Nanoparticles**
D Mei, Pacific Northwest National Laboratory, Richland, Washington
GA Henkelman, L Xu, RC Terrell, University of Texas at Austin, Austin, Texas

**First Principles Multiscale Analysis of Biochemical Processes: Signal Transduction and Spectroscopic Analysis of Local Structure-Folding Relations in Membrane Proteins**
MB Luskin, University of Minnesota, Minneapolis, Minnesota
JH Miller, Washington State University, Richland, Washington
PA Cole, Johns Hopkins University, Baltimore, Maryland
EJ Bylaska, TP Straatsma, Pacific Northwest National Laboratory, Richland, Washington
BM Elsasser, University of Paderborn, Paderborn, Germany
JC Mitchell, University of Wisconsin-Madison, Madison, Wisconsin
K Kowalski, M Valiev, EMSL, Richland, Washington
W E, Princeton University, Princeton, New Jersey

JH Weare, J Adams, SB Baden, JE Kim, PW Langhoff, JA Mccammon, SS Taylor, W Wang, SE Wong, EL Cauet, P Cheng, RP Daly, University of California, San Diego, La Jolla, California

**Formation of Apatite in Hanford Vadose Zone Sediments by Gaseous Injection of Phosphorus Compounds**
ML Rockhold, JE Szecsody, J McKinley, Pacific Northwest National Laboratory, Richland, Washington

**Free Radical Reactions in the Catalytic Cycle of Cytochrome bc Complexes**
DM Kramer, JL Cape, IP Forquer, Washington State University, Pullman, Washington
TP Straatsma, Pacific Northwest National Laboratory, Richland, Washington
M Valiev, EMSL, Richland, Washington
MK Bowman, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**FRET-Based Molecular Dynamics Simulation of Membrane-Receptor Activation**
G Orr, L Opresko, KJ Cassens, Pacific Northwest National Laboratory, Richland, Washington
K Wittrup, Massachusetts Institute of Technology, Cambridge, Massachusetts
HS Wiley, ER Vorpagel, EMSL, Washington

**From Activity to ORF**
DH Kohl, Washington University in St. Louis, St. Louis, Missouri

**From Gas Phase Clusters to Nanomaterials**
L Wang, W Huang, L Cui, H Zhai, Z Sun, X Xing, Washington State University, Richland, Washington
S Li, Xinzhou Teachers University, Xinzhou City, Shanxi, China
L Wang, Washington State University Tri-Cities, Richland, Washington
G Xiao, Xi'an Jiaotong University, Xi'an, Shaanxi, China

**Functional Interfaces at the Nanoscale**
JW Grate, MG Warner, G Exarhos, LM Bauder, Pacific Northwest National Laboratory, Richland, Washington
AJ Tyler, Utah State University, Logan, Utah
P Long, J Hu, Michigan State University, East Lansing, Michigan
MA Nash, PS Stayton, University of Washington, Seattle, Washington
T Weaver, Norfolk State University, Norfolk, Virginia

**Functional Materials for Separation and Sensing**
JT Bays, S Addleman, JW Grate, MG Warner, W Yantasee, CL Warner, Pacific Northwest National Laboratory, Richland, Washington
B Arey, MH Engelhard, EMSL, Richland, Washington

**Fundamental Investigations of Heterogeneous Catalysis Using Isotopic Transient Kinetic Analysis**
S Chuang, University of Akron, Akron, Ohio
RS Disselkamp, VM Lebarbier, Y Yang, CH Peden, Pacific Northwest National Laboratory, Richland, Washington
M White, Mississippi State University, Mississippi State, Mississippi
CT Campbell, L Cameron, IM Jensen, University of Washington, Seattle, Washington
J Goodwin, Clemson University, Clemson, South Carolina

C Mims, University of Toronto, Toronto, Ontario, Canada

**Fundamental Mechanistic Studies of Catalytic Hydrogen Production and Utilization**
CH Peden, Y Yang, J Szanyi, D Mei, Pacific Northwest National Laboratory, Richland, Washington
CT Campbell, University of Washington, Seattle, Washington
GA Henkelman, RC Terrell, University of Texas at Austin, Austin, Texas
C Mims, University of Toronto, Toronto, Ontario, Canada

**Fundamental Studies on Biomolecule Ions Desorbed from Open-Air Surfaces**
O Hadjar, Pacific Northwest National Laboratory, Richland, Washington
FM Fernandez, L Nyadong, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia
Z Yang, University of Colorado Boulder, Boulder, Colorado

**Fundamental Studies of Heterogeneous Photocatalysis on Model $TiO_2$ Surfaces**
MA Henderson, R Zehr, Pacific Northwest National Laboratory, Richland, Washington
Y Du, I Lyubinetsky, EMSL, Richland, Washington

**Fundamental Studies of Nitrogen Oxide Surface Chemistry: A Model System Approach**
Y Kim, Hanbat National University (formerly Taejon National University of Technology), Taejon, Korea South, Republic Of
J Szanyi, CH Peden, D Mei, Pacific Northwest National Laboratory, Richland, Washington
C Yi, Texas A&M University, College Station, Texas
I Lyubinetsky, EMSL, Richland, Washington
GA Henkelman, RC Terrell, University of Texas at Austin, Austin, Texas
F Netzer, Karl-Franzens-University Graz, Graz, Austria

**Fundamental Studies of Nitrogen Oxide Surface Chemistry: A Model System Approach Combining Experiments and Theory**
K Mudiyanselage, J Szanyi, J Kwak, Pacific Northwest National Laboratory, Richland, Washington
RC Terrell, University of Texas at Austin, Austin, Texas

**Fundamental Understanding of Charge Transfer from a Ru-Based Dye Adsorbate to a $TiO_2(110)$ Surface**
MA Henderson, Pacific Northwest National Laboratory, Richland, Washington
BA Parkinson, Colorado State University, Fort Collins, Colorado
T Thevuthasan, P Nachimuthu, EMSL, Richland, Washington

**Genomes-to-Life Protein Complex Isolation Capability**
BS Hooker, K Victry, D Auberry, C Lin, Pacific Northwest National Laboratory, Richland, Washington
HS Wiley, EMSL, Richland, Washington

**Global Cloud Resolving Model: Benchmarking, Data Access, and Model Testing**
KL Schuchardt, BJ Palmer, AS Koontz, J Piernas Canovas, JA Daily, Pacific Northwest National Laboratory, Richland, Washington
RJ Latham, Argonne National Laboratory, Argonne, Illinois
RP Heikes, DA Randall, DA Dazlich, Colorado State University, Fort Collins, Colorado

**Global Proteomic Analysis of Human Ehrlichiosis Agents**
Y Rikihisa, Ohio State University, Columbus, Ohio

**Glycolipid Structure, Dynamics and Recognition in a Membrane Environment**
RJ Woods, ML Demarco, MB Tessier, BY Austin, CR Daniels, University of Georgia, Athens, Georgia

**Grand Challenge in Biogeochemistry**
J Zachara, JK Fredrickson, Pacific Northwest National Laboratory, Richland, Washington
KH Nealson, University of Southern California, Los Angeles, California
AR Felmy, R Kukkadapu, EMSL, Richland, Washington

**Grand Challenge in Membrane Biology**
LA Sherman, T Summerfield, Purdue University, West Lafayette, Indiana
GW Buchko, JM Jacobs, Pacific Northwest National Laboratory, Richland, Washington
HB Pakrasi, BK Ghosh, Washington University in St. Louis, St. Louis, Missouri
R Kunnavakkam, R Aurora, Saint Louis University, St. Louis, Missouri
N Koropatkin, Donald Danforth Plant Science Center, St. Louis, Missouri
T Ogawa, Shanghai Institute of Plant Physiology and Ecology, Shanghai, China

**Grape Berry Shrivel: A Study of Anatomical and Ultrastructural Changes**
J Shutthanandan, BR Bondada, Washington State University, Richland, Washington

**Great Lakes Bioenergy Research Center**
MS Lipton, Pacific Northwest National Laboratory, Richland, Washington

**Gregory Szulczewski's Proposal**
GJ Szulczewski, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**Ground Squirrel Proteome: Protein Modifications through Torpor and Arousal**
LE Epperson, SL Martin, University of Colorado, Aurora, Colorado

**Growth Media Component Peptide and Carbohydrate Analysis**
KL Wahl, DS Wunschel, Pacific Northwest National Laboratory, Richland, Washington

**Growth of Single Crystal La$^2$CuO(4+delta) films**
SM Heald, Argonne National Laboratory, Argonne, Illinois

**Growth of Ti-Doped Epitaxial Alpha-$Fe_2O_3$(0001) Thin Films**
C Kim, Canadian Light Source Inc., Saskatoon, Saskatchewan, Canada

**Growth-Phase Regulation of the Proteome of *Rhodobacter capsulatus***
SJ Callister, Pacific Northwest National Laboratory, Richland, Washington
AS Lang, Memorial University of Newfoundland, St. John's, Newfoundland, Canada

**Heart Metabolomics during Ventricular Unloading**
OM Hyyti, University of Washington, Seattle, Washington
MA Portman, A Olson, Children's Hospital and Regional Medical Center, Seattle, Washington

**Heterogeneous Photochemistry of Organic-Coated Mineral Dust Aerosol**
VH Grassian, MA Young, OB Laskina, University of Iowa, Iowa City, Iowa

A Laskin, EMSL, Richland, Washington

**Heterogeneous Uptake of $HNO_3$ on $CaCO_3$: Determination of the Gas-Particle Reaction Probability as Function of Relative Humidity**
VH Grassian, ER Gibson, OB Laskina, University of Iowa, Iowa City, Iowa
JP Cain, H Wang, University of Southern California, Los Angeles, California
A Laskin, EMSL, Richland, Washington
Y Liu, University of California, San Diego, La Jolla, California

**High Accuracy Modeling of Frequency Dependent Polarizabilities: Exploring the Cutting Edge Limits of NWChem**
JR Hammond, University of Chicago, Chicago, Illinois
PJ Nichols, EJ Bylaska, Pacific Northwest National Laboratory, Richland, Washington
WA De Jong, Kn Kowalski, M Valiev, D Wang, N Govind, KR Glaesemann, EMSL, Richland, Washington

**High-Field Static QCPMG $^{47}$Ti and $^{49}$Ti Studies of Nanoparticulate $TiO_2$**
SE Hayes, Washington University in St. Louis, Saint Louis, Missouri

**High-k Oxides and Their Mixed Oxide Systems**
CV Ramana, University of Texas at El Paso, El Paso, Texas

**High-Performance Computing to Evaluate Hierarchical Heterogeneity Paradigms in Sedimentary Aquifer Systems**
TD Scheibe, VL Freedman, Pacific Northwest National Laboratory, Richland, Washington
RW Ritzi, R Ramanathan, A Guin, Wright State University, Dayton, Ohio

**High Performance Sequence Analysis for Data-Intensive Bioinformatics**
CS Oehmen, L McCue, Pacific Northwest National Laboratory, Richland, Washington
HJ Sofia, Whitman College, Walla Walla, Washington
EA Welsh, Washington University in St. Louis, St. Louis, Missouri
DJ Baxter, EMSL, Richland, Washington

**High-Performance Support Vector Machines for Data-Intensive Applications**
BM Webb-Robertson, CS Oehmen, Pacific Northwest National Laboratory, Richland, Washington

**High Pressure VLS Synthesis of Silicon Nanowires**
JC Chan, SB Rananavare, Portland State University, Portland, Oregon

**High Pressure VLS Synthesis of Silicon Nanowires**
SB Rananavare, JC Chan, Portland State University, Portland, Oregon

**High Resolution $^{1}$H NMR Metabolomics Using Slow and Ultra Slow Magic Angle Spinning**
Q Zhang, TO Metz, J Hu, KR Minard, M Murphy, K Thrall, A Woodstock, Pacific Northwest National Laboratory, Richland, Washington
D Rommereim, J Sears, EMSL, Richland, Washington
J Caceres-Cortes, Bristol-Myers Squibb, Lawrenceville, New Jersey

**High-Resolution $^{27}$Al and $^{133}$Cs NMR of Weathered Hanford Sediments**

KT Mueller, CR Strepka, C Fleeger, Pennsylvania State University, University Park, Pennsylvania

**High Resolution Electron Microscopy Study of Nanostructured Materials**
J Liu, K Zhu, D Wang, Z Nie, R Kou, D Choi, Pacific Northwest National Laboratory, Richland, Washington
D Liu, University of Washington, Seattle, Washington

**High Resolution Fourier Transform Infrared Spectroscopy Studies of Multidimensional H Transfer in Tropolone/Tropolonoid Molecules-a Bridge to the Behavior in Biological Systems**
TA Blake, RL Sams, Pacific Northwest National Laboratory, Richland, Washington
RL Redington, Texas Tech University, Lubbock, Texas

**High-Resolution Magic Angle Spinning NMR Spectroscopy of Microtubule-Associated Motor Proteins**
Y Han, TE Polenova, S Sun, S Paramasivam, University of Delaware, Newark, Delaware

**High Resolution TEM of Doped Ceria System**
S Omar, JC Nino, University of Florida, Gainesville, Florida

**High Temperature, Large Sample Volume, Constant Flow Magic Angle Spinning NMR Probe for 11.7 T Magnetic Field for In-situ Catalytic Reaction Characterization**
J Hu, Pacific Northwest National Laboratory, Richland, Washington
JJ Ford, J Sears, EMSL, Richland, Washington

**High-Throughput Evaluation of Breast Cancer Markers**
RC Zangar, Pacific Northwest National Laboratory, Richland, Washington

**High Throughput Proteomic & Metabolomic Early Biomarkers (PNNL Scope #47174, RD Smith's EIF project)**
T Liu, RD Smith, DG Camp, MA Gritsenko, Pacific Northwest National Laboratory, Richland, Washington

**Host Cell Interactions with Human Infectious Diseases, Straub**
K Honer Zu Bentrup, Tulane University, New Orleans, Louisiana
TM Straub, CO Valdez, R Bartholomew, CJ Bruckner-Lea, Pacific Northwest National Laboratory, Richland, Washington
CP Gerba, P Orosz Coglhan, University of Arizona, Tucson, Arizona
A Dohnalkova, B Arey, EMSL, Richland, Washington
C Nickerson, Arizona State University, Tempe, Arizona
J Vinje, Center for Disease Control Prevention, Atlanta, Georgia
S Fout, Environmental Protection Agency, Cincinnati, Ohio

**Hybrid Numerical Methods for Multiscale Modeling of Subsurface Biogeochemical Processes**
G Lin, BJ Palmer, TD Scheibe, Y Fang, AM Tartakovsky, GE Hammond, L Sun, GD Black, JM Chase, KL Schuchardt, TO Elsethagen, VL Freedman, HE Trease, JA Fort, WA Perkins, H Silva, JA Daily, Pacific Northwest National Laboratory, Richland, Washington
BA Allan, Sandia National Laboratory, Livermore, California

**Hydrogen Bonding in Inhomogeneous Environments**

SI Sukharev, AG Anishkin, University of Maryland, College Park, Maryland
ME Green, VS Znamenskiy, S Liao, City College of New York, New York, New York
M Mezei, Mount Sinai School of Medicine, New York, New York

**Hydrogen Materials Compatibility Studies**
CH Henager, JD Holbery, KJ Alvine, Pacific Northwest National Laboratory, Richland, Washington

**Hydrogen Production-(Steam Reforming of hydrocarbons Including Methane, Propane, Gasoline, Jet Fuel and Biomass Derived Products)**
J Hu, RA Dagle, D Howe, B Roberts, CM Fischer, G Whyatt, VM Lebarbier, A Karim, J Sun, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, B Arey, EMSL, Richland, Washington
AB Kazi, KL Durand, AV Lyles, University of Arkansas at Pine Bluff, Pine Bluff, Arkansas

**Hydrogenation of Pyrolysis Oils to Create Gasoline**
T Hart, D Elliott, Pacific Northwest National Laboratory, Richland, Washington

**Hydronium Hydroxide at Platinum Interfaces**
JP Cowin, Pacific Northwest National Laboratory, Richland, Washington
Y Lilach, Hebrew University of Jerusalem, Jerusalem, Israel
M Iedema, EMSL, Richland, Washington
AM Endres, Central Washington University, Ellensburg, Washington

**Hygroscopic Properties of Aerosol Organics**
A Zelenyuk, R Zaveri, J Yang, Pacific Northwest National Laboratory, Richland, Washington
AG Hallar, DH Lowenthal, Desert Research Institute, Reno, Nevada

**Ice Nucleation on Aged Field Aerosols**
JP Cowin, HM Ali, X Yu, Pacific Northwest National Laboratory, Richland, Washington
M Iedema, EMSL, Richland, Washington

**Identification and Characterization of Soluble Factors in Delayed Effects of Low Dose Radiation**
DL Springer, Pacific Northwest National Laboratory, Richland, Washington

**Identification and Validation of Protein Profiles Associated with Therapy-Resistance in Breast Cancer**
L Pasa-Tolic, EMSL, Richland, Washington
A Umar, TM Luider, JA Foekens. Erasmus University Medical Center, Rotterdam, Rotterdam, Netherlands

**Identification of Precipitates and Chemistry of Interfaces in Optical Materials**
DF Bahr, A Bellou, MM Reynolds, Washington State University, Pullman, Washington

**Identify Biomarkers for COPD (Chronic Obstructive Pulmonary Disease) in Humans Using Proteomic and Metabonomic Analysis of Serum and Urine**
SM Varnum, J Pounds, Pacific Northwest National Laboratory, Richland, Washington

**Identify Morphology of Initial LIGO Core Optics Scatter Sites**
G Billingsley, California Institute of Technology, Pasadena, California

CA Vorvick, California Institute of Technology/Jet Propulsion Laboratory/NASA, Richland, Washington

**Identifying Targets for Therapeutic Interventions using Proteomic Technology**
JN Adkins, KD Rodland, N Manes, S Chowdhury, Pacific Northwest National Laboratory, Richland, Washington
HM Mottaz, EMSL, Richland, Washington
F Heffron, S Wong, R Estep, Oregon Health Sciences University/Oregon Graduate Institute, Portland, Oregon

**Imaging of a Solid Oxide Fuel Cell Cathode**
EM Ryan, C Amon, Carnegie Mellon University, Pittsburgh, Pennsylvania

**Imaging of Water and Gas Distribution in PEM Fuel Cell Stacks and Cells**
KR Minard, L Wang, PD Majors, VV Viswanathan, PC Rieke, Pacific Northwest National Laboratory, Richland, Washington

**Imaging Respiratory Structure and Function in Laboratory Animals**
KR Minard, RA Corley, C Timchalk, R Jacob, Pacific Northwest National Laboratory, Richland, Washington

**Immiscibility Features between Silica-Rich and Carbonate-Rich Material in Breccia from the Sierra Madera Impact Structure**
SA Huson, MC Pope, Washington State University, Pullman, Washington

**Impact of Reactive Halogen Species on the Air Quality in Southern California Coastal Areas**
MH Erickson, BT Jobson, J McCoskey, Washington State University, Pullman, Washington
JP Stutz, University of California, Los Angeles, Los Angeles, California
A Laskin, EMSL, Richland, Washington
Y Liu, University of California, San Diego, La Jolla, California

**Implications of U Sequestration in U-Al-$SO_4$-Si Grain Coatings for Remediation and Stewardship**
AS Madden, BP Spalding, Oak Ridge National Laboratory, Oak Ridge, Tennessee
D Phillips, Queen's University Belfast, Belfast, Ireland
DE Watson, ElSohly Laboratories, Inc., Oxford, Mississippi

**Improving the Execution Time of NWLang**
H Resat, Pacific Northwest National Laboratory, Richland, Washington
KA Glass, EMSL, Richland, Washington

**Impurity Segregation and Precipitation in Semiconductor Nanostructures**
ST Dunham, BC Trzynadlowski, W Jiang, L Lin, H Lai, University of Washington, Seattle, Washington

***In-situ* Electron Microscopy and Spectroscopy Studies of Interfaces in Advanced Li-Ion Batteries under Dynamic Operation Conditions**
Z Yang, J Liu, Pacific Northwest National Laboratory, Richland, Washington
T Thevuthasan, C Wang, EMSL, Richland, Washington

**Incorporation of Cellulose Nanocrystals into PHB/PHV Copolymer**

MP Wolcott, Washington State University, Pullman, Washington
JD Holbery, Pacific Northwest National Laboratory, Richland, Washington
Y Lao, unknown, unknown, Washington

**Inelastic Electron Scattering Cross Section Measurements in Liquid Water**
NG Petrik, RG Tonkyn, GA Kimmel, Pacific Northwest National Laboratory, Richland, Washington
CM Brown, Wadsworth Center, Albany, New York

**Influence of Microscopic Mass Transfer on the Reactivity and Stability of Uranium**
C Liu, Z Wang, J Zachara, Pacific Northwest National Laboratory, Richland, Washington
RP Ewing, Iowa State University, Ames, Iowa

**Infrared Adiabatic Rapid Passage Spectroscopy of Small Gas Phase Molecules**
TA Blake, J Kelly, Pacific Northwest National Laboratory, Richland, Washington
KA Glass, EMSL, Richland, Washington

**Infrared Absorption Cross Sections of Acetone and Acetic Acid**
A Weber, National Institute of Standards and Technology, Gaithersburg, Maryland

**Infrared Reflectance Spectroscopy of Soils (Blake's NNSA, PNNL Scope #43865)**
TA Blake, Pacific Northwest National Laboratory, Richland, Washington
PL Gassman, EMSL, Richland, Washington

**Infrared Spectroscopy of Methyl Halides (Blake's LDRD, PNNL Scope #49961)**
TA Blake, TJ Johnson, Pacific Northwest National Laboratory, Richland, Washington

**Innovative Aerosol Collector (Alexander's SBIR, PNNL Scope #48595)**
R Zaveri, Pacific Northwest National Laboratory, Richland, Washington
D Worsnop, JT Jayne, Aerodyne Research Inc, Billerica, Massachusetts

**Instrument Testing and Deployment for the DOE CHAPS Field Campaign**
CM Berkowitz, R Zaveri, Pacific Northwest National Laboratory, Richland, Washington
L Alexander, EMSL, Richland, Washington
JA Ogren, National Oceanic and Atmospheric Administration (NOAA), Boulder, Colorado

**Integrated Experimental and Modeling Studies on Aerosol Evolution and Aging**
R Zaveri, RC Easter, A Zelenyuk, J Yang, C Song, Pacific Northwest National Laboratory, Richland, Washington
L Alexander, EMSL, Richland, Washington

**Integrated Experimental and Modeling Studies on Secondary Organic Aerosol Formation**
R Zaveri, SM Kathmann, A Zelenyuk, DA Maughan, JC Birnbaum, J Yang, C Song, Pacific Northwest National Laboratory, Richland, Washington
S Madronich, National Center for Atmospheric Research, boulder, Colorado
A Laskin, EMSL, Richland, Washington
JA Thornton, University of Washington, Seattle, Washington

**Integrated NMR/SIP Technologies for the Functional and Structural Characterization of Microbial Communities**

PD Majors, JC Scholten, J McLean, Pacific Northwest National Laboratory, Richland, Washington

**Integrated Top-Down and Bottom-Up Proteomics Strategy to Identify Multisite and Multistep Modifications on Radiation Sensitive Proteins**
DL Stenoien, Pacific Northwest National Laboratory, Richland, Washington

**Interactions Between Domains in Dematin, a Key Component of the Red Blood Cell Junctional Complex**
CJ Mcknight, Boston University School of Medicine, Boston, Massachusetts

**Interfaces and Interactions: Non-ideal Behavior of Biological Molecules**
W Chiu, EL Zechiedrich, Baylor College of Medicine, Houston, Texas
BM Pettitt, SL Johnsson, R Glowinski, TE Warth, GC Lynch, K Wong, KM Dyer, C Chen, JS Perkyns, W Li, JJ Howard, GL Randall, CY Hu, J Feng, H Kokubo, JG Reid, B Lin, Y Bai, University of Houston, Houston, Texas

**Interfacial Excited State Dynamics on $TiO_2$**
WP Hess, Pacific Northwest National Laboratory, Richland, Washington
K Tanimura, Osaka University, Osaka, Japan
KM Beck, EMSL, Richland, Washington

**Interfacial Phenomena in Cu Plating**
VM Dubin, Y Tao, J Blanchard, X Xu, L Maretti, K Agapiou, eMAT Technology LLC, Moses Lake, Washington

**Interrogation of Glucose Metabolism by Oral Biofilms Using Combined NMR/Optical Spectroscopy and Stable Isotope Labeling**
JC Scholten, J McLean, PD Majors, Pacific Northwest National Laboratory, Richland, Washington

**Investigating Post-Translational Modifications of Kinesin**
SP Gross, University of California, Irvine, Irvine, California

**Investigating the Correlation Among Properties, Morphology and Composition of Multimetallic Alloy and Core-shell Nanoparticles and Novel Nanostructures**
C Zhong, P Njoki, D Mott, S Lim, State University of New York at Binghamton, Binghamton, New York
MH Engelhard, EMSL, Richland, Washington

**Investigation of Arsenic and Lead Migration at Former Phosphate Fertilizer Plants**
KJ Cantrell, W Deutsch, Pacific Northwest National Laboratory, Richland, Washington
B Arey, EMSL, Richland, Washington

**Investigation of Dynamics of Villin Headpiece Subdomain by Solid-State NMR with the Use of Single-Site Labeling**
AS Lipton, Pacific Northwest National Laboratory, Richland, Washington
JJ Ford, EMSL, Richland, Washington
L Vugmeyster, University of Alaska at Anchorage, Anchorage, Alaska

**Investigation of the Metal Binding Octarepeat Region from the Human Prion using Nanoscale Computer Simulations**

DJ Doren, RH Wood, O Rahaman, University of Delaware, Newark, Delaware
EM Yezdimer, Industrial Summit Technology, Parlin, New Jersey

**Investigation of Water-Soluble X-ray Luminescence Nanoparticles for Biomedical Applications**
W Chen, University of Texas at Arlington, Arlington, Texas

**Investigations into Sulfur Poisoning Mechanisms in Solid-State Oxide Fuel Cells Using Quantum-Chemical Computations**
M Liu, J Wang, Y Choi, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia

**Investigations of Electric Field Gradients and NMR Chemical Shifts of $^{87}$Sr in Mixed Calcium/Strontium Systems Using High Field NMR and Computational Chemistry**
KT Mueller, Pennsylvania State University, University Park, Pennsylvania

**Ion Beam Analysis of Components for Solid Oxide Fuel Cells**
RJ Smith, M Finsterbusch, Montana State University, Bozeman, Montana
CV Ramana, University of Texas at El Paso, El Paso, Texas

**Ion Beam Implantation of Titanium Alloys to Improve Durability in Structural and Biomedical Applications**
MP Carroll, Washington State University, Pullman, Washington
KO Findley, Colorado School of Mines, Golden, Colorado

**Ion Beam Methods for the Synthesis, Modification, and Characterization of Radiation Detection Materials**
L Boatner, JS Neal, Oak Ridge National Laboratory, Oak Ridge, Tennessee

**Ion Channeling Studies of Epitaxial Oxide Films and Gas-Solid Interfaces**
KR Padmanabhan, Wayne State University, Detroit, Michigan

**Ionic Transport of Hydrogen in Structured Soft Materials**
JP Cowin, Pacific Northwest National Laboratory, Richland, Washington
M Iedema, EMSL, Richland, Washington
K Wu, Peking University, Beijing, China
RC Bell, Pennsylvania State University, Altoona, Pennsylvania

**Irradiation Induced Nanostructures**
L Wang, X Xiang, H Xiao, University of Michigan, Ann Arbor, Michigan

**Isoform-Specific Quantitative Proteomics Applying N-terminal Enrichment and Informatics Deconvolution**
W Qian, BO Petritis, Pacific Northwest National Laboratory, Richland, Washington

**Kiln Phosphoric Acid (KPA) Process**
T Hart, Pacific Northwest National Laboratory, Richland, Washington
JA Megy, JDC, Inc, New Cumberland, West Virginia

**Kinetic Study of Heterogeneous Reaction of Soot with Reactive Oxidants**
H Wang, JP Cain, University of Southern California, Los Angeles, California
C Wang, A Laskin, PL Gassman, EMSL, Richland, Washington

Y Liu, University of California, San Diego, La Jolla, California

**Laboratory Spectroscopy of $CO_2$ for Earth Observations**
TA Blake, RL Sams, Pacific Northwest National Laboratory, Richland, Washington
MA Smith, NASA Langley Research Center, Hampton, Virginia

**Laser Desorption from Metal Oxides**
PV Sushko, AL Shluger, London, University College, London, United Kingdom
WP Hess, AG Joly, Pacific Northwest National Laboratory, Richland, Washington
KM Beck, EMSL, Richland, Washington
MJ Wolf, University College London, London, United Kingdom

**LC-FTMS Analysis of Organophosphates**
CG Fraga, Pacific Northwest National Laboratory, Richland, Washington

**LC-FTMS Analysis of Parathion, Dichlor, and TETS**
CG Fraga, Pacific Northwest National Laboratory, Richland, Washington

**LC-MS-Based Metabolomics for Computational Toxicology**
TO Metz, A Miracle, DW Koppenaal, Pacific Northwest National Laboratory, Richland, Washington
D Ekman, T Collette, Environmental Protection Agency, Athens, Georgia

**Lignin and Depolymerised Lignin Characterization by High Performance liquid Chormotography Mass Spectrometry (LCMS)**
R Zhang, EMSL, Richland, Washington

**Linking Microscopic to Macroscopic Adsorption/Desorption Behavior for Uranium on Environmental Materials**
KM Rosso, SC Smith, ES Ilton, O Qafoku, J Friese, P Bachelor, Pacific Northwest National Laboratory, Richland, Washington

**Lirong Zhong's Proposal -- TEM/SEM-Microprobe Study on Carbon Dioxide Flooding Sandstone Core**
L Zhong, Pacific Northwest National Laboratory, Richland, Washington
SL Patil, University of Alaska, Fairbanks, Fairbanks, Alaska

**Local Structure in Zirconia-Based Nuclear Fuels and Transmutation Targets**
I Farnan, University of Cambridge, Cambridge, United Kingdom
J Somers, European Commission Joint Research Centre, Karlsruhe, Germany, Germany

**Location and Interactions of Vanadium-Containing Probes in a Model Membrane System**
MA Sedgwick, DC Crans, B Baruah, Colorado State University, Fort Collins, Colorado

**Location of Probes in Membrane and Model Membrane Systems and Their Effects on Lipid Reorganization**
MA Sedgwick, DC Crans, B Baruah, E Gaidamauskas, AM Trujillo, Colorado State University, Fort Collins, Colorado

**Longitudinal Proteomic Characterization of Human Cerebrospinal Fluid**

DG Camp, SO Purvine, T Liu, Pacific Northwest National Laboratory, Richland, Washington
SE Schutzer, University of Medicine and Dentistry, New Jersey Medical School, Newark, New Jersey

**Low Temperature (10K) $^{25}$Mg Solid-State NMR of DNA Repair Proteins and Their Complexes**
PD Ellis, AS Lipton, R Heck, Pacific Northwest National Laboratory, Richland, Washington
DM Wilson, National Institute on Aging, IRP, NIH, Baltimore, Maryland
SH Wilson, National Institute of Environmental Health Sciences, NIH, RTP, North Carolina

**Lustre Scalability Research**
EJ Felix, DM Brown, EMSL, Richland, Washington
B Schroeder, University of Toronto, Toronto, Ontario, Canada

**Magnetic Resonance Microscopy of Ozone-Induced Lung Injury**
KR Minard, RA Corley, R Jacob, Pacific Northwest National Laboratory, Richland, Washington

**Maria Salazar-Villalpando's Proposal**
MD Salazar-Villalpando, DA Berry, National Energy Technology - Laboratory, Morgantown, West Virginia

**Material Homogeneity Studies on 3D Microfabricated Ceramic Structures Using Nanoparticle Building Blocks**
SV Atre, Oregon State University, Corvallis, Oregon

**Material Interactions at Interfaces in Solid Oxide Fuel Cells**
JS Hardy, VL Sprenkle, KD Meinhardt, J Kim, NL Canfield, JF Bonnett, Pacific Northwest National Laboratory, Richland, Washington

**MBE Growth and Properties of Model $TiO_2$ Surfaces for Fundamental Studies of Heterogeneous Photocatalysis**
SA Chambers, MA Henderson, T Ohsawa, Pacific Northwest National Laboratory, Richland, Washington
C Wang, P Nachimuthu, Y Du, EMSL, Richland, Washington
R Shao, unknown, Washington

**MBE Growth and Properties of N-doped $TiO_2$ for Enhanced Visible Light Absorption and Water Splitting**
SA Chambers, S Cheung, MA Henderson, T Ohsawa, Pacific Northwest National Laboratory, Richland, Washington
SM Heald, Argonne National Laboratory, Argonne, Illinois
J Rodriguez, Brookhaven National Laboratory, Upton, New York
C Wang, P Nachimuthu, V Shutthanandan, EMSL, Richland, Washington
CS Fadley, Lawrence Berkeley National Laboratory, Richland, West Virginia

**Measurement and Optimization of the Redox Properties of Enzymes Using Single-Molecule Imaging, Controlled Electrochemical Potential, and Nanoscale Confinement**

EJ Ackerman, D Hu, C Lei, C Windisch, Pacific Northwest National Laboratory, Richland, Washington

**Measurement of Ambient Concentrations of Aerosols to Support the Analysis of MIRAGE Urban Plume Transport and Chemistry**
JL Jimenez, University of Colorado, Boulder, Colorado
BK Lamb, R Grivicke, Washington State University, Pullman, Washington

**Measurement of Saturation-Dependent Anisotropy in Hydraulic Conductivity of Hanford Vadose Zone Sediments**
F Zhang, Pacific Northwest National Laboratory, Richland, Washington

**Measuring Nanometer Distances in the Packaging RNA using Double Electron-Electron Resonance**
PZ Qin, Q Cai, GG Grant, A Popova, University of Southern California, Los Angeles, California
MK Bowman, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**Mechanisms of Laser and Electron Beam Modifications of Wide Bandgap Single Crystal Surfaces**
JT Dickinson, E Khan, Washington State University, Pullman, Washington
WP Hess, Pacific Northwest National Laboratory, Richland, Washington

**Mechanisms of Ubiquitin Transfer and Regulation**
PS Brzovic, R Klevit, D Fox, DM Wenzel, CM Eakin, C Heikaus, University of Washington, Seattle, Washington

**Mechanistic Studies of Protein Allostery at the Atomistic Scale**
J Chu, JB Brokaw, University of California, Berkeley, Berkeley, California

**Metabolomics and Proteomics of Bacterial Signaling**
OM Mcdougal, K Cornell, Boise State University, Boise, Idaho

**Metal-Induced Crystallization Via Sputtering Deposition on Flexible Substrates and Its Applications**
ST Dunham, C Shih, H Guo, University of Washington, Seattle, Washington

**Michael Knoblauch's Proposal, Molecular Structure and Interaction of Forisome Filaments**
M Knoblauch, DR Froelich, Washington State University, Pullman, Washington

**Microbiological, Geochemical and Hydrologic Processes Controlling Uranium Mobility: An Integrated Field-Scale Subsurface Research Challenge Site at Rifle, Colorado**
R Kukkadapu, C Wang, EMSL, Richland, Washington

**Microfabrication of Electrospray Emitter Arrays For Improved Sensitivity in Electrospray Ionization-Mass Spectrometry**
RT Kelly, RD Smith, K Tang, Pacific Northwest National Laboratory, Richland, Washington

**Microsampling Isotope Ratio Mass Spectrometer Development**

R Zaveri, A Mendoza, RA Dagle, BR Johnson, HW Kreuzer, DJ Gaspar, Pacific Northwest National Laboratory, Richland, Washington

**Microscale and Spectroscopic Investigations in Geochemical and Microbiological Systems**
J Zachara, J McKinley, ES Ilton, KM Rosso, Z Wang, C Liu, M Oostrom, DA Moore, MA Covert, TE Queen, Pacific Northwest National Laboratory, Richland, Washington
R Kukkadapu, A Dohnalkova, TW Wietsma, B Arey, PL Gassman, EMSL, Richland, Washington
J Boily, Umea University, Umea, Sweden
BH Lower, The Ohio State University, Columbus, Ohio

**Microscopic Mass Transfer on U(VI) and Tc(VIII) in Subsurface sediments**
C Liu, Z Wang, Pacific Northwest National Laboratory, Richland, Washington
RP Ewing, Iowa State University, Ames, Iowa

**Microscopy Investigation on Nanostructured Electrodes**
J Zhang, D wang, G Xia, J Liu, W Xu, Pacific Northwest National Laboratory, Richland, Washington

**Mitotic Regulation of the Nuclear Pore Complex Protein Interaction Network**
SA Osmani, Ohio State University, Columbus, Ohio
R Zhao, EMSL, Richland, Washington

**Mixed Oxide Films for Gas Sensing and Photo-Catalytic Applications**
KR Padmanabhan, Wayne State University, Detroit, Michigan

**Model Development on Using Clay Membranes for Arsenic Removal from Drinking Water**
C Liu, Pacific Northwest National Laboratory, Richland, Washington
B Deng, University of Missouri, Columbia, Columbia, Missouri

**Model Oxide Defects with Vicinally Stepped NiO(100) Substrates**
Y Du, I Lyubinetsky, EMSL, Richland, Washington
MA Langell, University of Nebraska, Lincoln, Nebraska

**Model System Surface Science Approach to Study Photochemistry at Adsorbate-Substrate Interfaces: The Trimethyl Acetate, Silver, Titania System**
MA Henderson, Z Dohnalek, Pacific Northwest National Laboratory, Richland, Washington
I Lyubinetsky, EMSL, Richland, Washington
JM White. University of Texas at Austin, Austin, Texas
SC Andrews, unknown, Washington

**Modeling Charge Transport and Interfacial Chemistry at the Nanoscale**
R Devanathan, Pacific Northwest National Laboratory, Richland, Washington
PA Moreira, Universidade Estadual De Campinas, Sao Paulo, Brazil

**Modeling Multiscale-Multiphase-Multicomponent Subsurface Reactive Flows using Advanced Computing**
GE Hammond, Pacific Northwest National Laboratory, Richland, Washington
PC Lichtner, Los Alamos National Laboratory, Los Alamos, New Mexico
RT Mills, Oak Ridge National Laboratory, Oak Ridge, Tennessee

**Modeling of Polymer Membrane Nanostructure and Its Effect on Proton and Small Molecule Transport**
R Devanathan, V Glezakou, M Dupuis, S Morrison-Smith, K Artiga, Pacific Northwest National Laboratory, Richland, Washington
A Venkatnathan, Indian Institute of Science Education and Research, Pune, Pune, Washington, India

**Molecular Beam Scattering Measurements on Anatase $TiO_2$(001) and Rutile $TiO_2$(110)**
U Burghaus, North Dakota State University, Fargo, North Dakota

**Molecular Computational Studies in Geochemistry and Environmental Chemistry**
JR Rustad, WH Casey, University of California, Davis, Davis, California
KM Rosso, SN Kerisit, EJ Bylaska, GK Schenter, M Dupuis, PJ Nichols, Pacific Northwest National Laboratory, Richland, Washington
M Valiev, EMSL, Richland, Washington
DA Dixon, VE Jackson, MT Nguyen, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
JH Weare, SA Bogatko, EL Cauet, University of California, San Diego, La Jolla, California

**Molecular Dynamics Study of an Actin Septamer: Testing the Holmes Model and the Hydrophobic Plug Loop Hypothesis**
GC Schatz, KM Barrett, MJ McCullagh, JT Paci, Northwestern University, Evanston, Illinois
KC Holmes, Max Planck Institut fur medizinische Forschung, Heidelberg, Germany

**Molecular Interfaces to Single-Crystal Anatase Surfaces**
RJ Hamers, University of Wisconsin-Madison, Madison, Wisconsin

**Molecular Level Construction of Functional Surfaces**
PL Gassman, EMSL, Richland, Washington
SM Gorun, LA Lapok, New Jersey Institute of Technology, Newark, New Jersey

**Molecular-Level Mechanisms of Microbial Basalt Alteration**
AS Templeton, University of Colorado, Boulder, Colorado
H Staudigel, University of California, San Diego, La Jolla, California
BM Tebo, Oregon Health Sciences University/Oregon Graduate Institute, Portland, Oregon

**Molecular-Level Understanding of Transport and Optic Properties of Doped Oxide Nanoclusters**
Y Qiang, J Antony, M Faheem, A Sharma, University of Idaho, Moscow, Idaho
C Wang, EMSL, Richland, Washington

**Molecular Mechanisms Underlying Cellular Adaptive Response to Low Dose Radiation**
CA Sacksteder, TC Squier, MA Gritsenko, Pacific Northwest National Laboratory, Richland, Washington

**Morphology, Composition and Surface Properties of Novel Functional Multimetallic and Core-Shell Nanoparticles and Assemblies**
C Zhong, State University of New York at Binghamton, Binghamton, New York

**Mössbauer Analysis of Microbial Redox Transformations of Naturally Occurring Fe(III)-Bearing Phyllosilicates**
EE Roden. University of Wisconsin, Madison, Wisconsin
ES Shelobolina, University of Wisconsin-Madison, Madison, Wisconsin
R Kukkadapu, EMSL, Richland, Washington

**Mossbauer and XPS Characterization of Fe-Based Fischer-Tropsch Catalysts**
R Kukkadapu, EMSL, Richland, Washington
V Subramani, Research Triangle Institute, Research Triangle Park, North Carolina

**Mössbauer Spectroscopy and SEM/TEM Study of the Reductive Dissolution of Fe-Oxyhydroxides in Porous Media**
CI Steefel, L Yang, Lawrence Berkeley National Laboratory, Berkeley, California

**MRI of Chronic Obstructive Pulmonary Disease**
KR Minard, C Timchalk, Pacific Northwest National Laboratory, Richland, Washington
KM Gideon, Battelle Columbus, Richland, Washington

**Multidimensional High-Field Magic-Angle Spinning NMR of Membrane and Nanocrystalline Proteins**
CM Rienstra, AJ Nieuwkoop, LJ Sperling, University of Illinois at Urbana-Champaign, Urbana, Illinois
L Mueller, Bristol-Myers Squibb, Princeton, New Jersey

**Multifunctional Nanostructures for Nano-Biotechnology Applications**
A Punnoose, MR Kongara, AP Thurber, Boise State University, Boise, Idaho

**Nano- and Atomic-Level Engineered Adsorbent, Catalyst, and Membrane Materials for Energy and Environmental Application**
A Karim, W Liu, XS Li, Y Su, H Wan, J Zhang, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington

**Nanomaterials for Chelation Therapies and Sensing Applications**
W Yantasee, D Choi, A Cinson, Pacific Northwest National Laboratory, Richland, Washington
T Sangvanich, K Pattamakomsan, B Charnhattakorn, V Koonsiripaiboon, J Kanlayanatham, V Sukwarotwat, Chulalongkorn University, Bangkok, Thailand

**Nanoparticle-Cell Interactions and Intracellular Fate; Roles of Particle Surface Properties**
BL Maddux, University of Oregon, Eugene, Oregon
KJ Cassens, G Orr, Pacific Northwest National Laboratory, Richland, Washington

**Nanoparticles-Based Biosensors for Detection of Environmental Biomarkers**
Y Miao, Portland State University, Portland, Oregon
CM Wai, K Shimizu, University of Idaho, Moscow, Idaho
Y Lin, C Timchalk, G Liu, H Wu, J Wang, RC Barry, J Liu, SL Riechers, X Zhang, Z Tang, D Choi, H Wang, A Ma-ham, Pacific Northwest National Laboratory, Richland, Washington
H Liao, Xiamen University, Xiamen, Fujian, China
H Nian, National Tsing Hua University, Hsingchu, Taiwan, Province Of China
K Pinwattana, Chulalongkorn University, Patuwan, Bangkok, Thailand

A Lee, National University of Singapore, Singapore, Malaysia
MH Engelhard, EMSL, Richland, Washington
D Du, Central China Normal University, Wuhan, Hubei, China
X Kang, Guangdong Ocean University, Guangdong, China
S Zhang, Harbin Institute of Technology, Harbin, China
Y Zhang, Hunan Normal University, Changsha, Hunan, China

**Nanoscale Characterization of Nanomaterial - Cell Interactions**
G Orr, BJ Tarasevich, J Teeguarden, J Pounds, JL Phillips, DJ Panther, ME Rosbach, KJ Cassens, Pacific Northwest National Laboratory, Richland, Washington

**Nanoscale Enzyme Reactors (NERs) for Biofuel Cells**
P Wang, University of Minnesota, Minneapolis, Minnesota
SY Ha, MB Fischback, Washington State University, Pullman, Washington
J Kim, Pacific Northwest National Laboratory, Richland, Washington
S Shin, K Kwon, H Park, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea South, Republic Of

**(gc3564)Nanostructure Formation, Aggregation, and Reactivity**
S Irle, Z Wang, B Finck, PN Bobadova-Parvanova, A Altun, I Kerkines-Keramidas, Emory University, Atlanta, Georgia
K Morokuma, Kyoto University, Kyoto, Japan
R Rousseau, M Dupuis, X Wang, SN Kerisit, EJ Bylaska, NA Deskins, D Mei, Pacific Northwest National Laboratory, Richland, Washington
F Mehmood, LA Curtiss, P Zapol, SP Adiga, MG Sternberg, H Iddir, JP Greeley, D Torres Rangel, Argonne National Laboratory, Argonne, Illinois
M Valiev, N Govind, EMSL, Richland, Washington
MA Langell, University of Nebraska, Lincoln, Nebraska
G Zheng, University of Illinois at Urbana-Champaign, Urbana, Illinois

**NBACC: Host/Pathogen Interactions (PNNL Scope # 49488, Lipton's NBACC Host Project)**
MS Lipton, Pacific Northwest National Laboratory, Richland, Washington
KK Hixson, EMSL, Richland, Washington

**Near Real-Time Alkene Sensor for Atmospheric Aerosol Chemistry Monitoring**
JW Grate, Pacific Northwest National Laboratory, Richland, Washington
R Shekarriz, MicroEnergy Technologies, Inc., Portland, Oregon

**Nerve Agent Detection Using Enzyme-Coated Nanowires**
Y Koo, S Lee, Inha University, Incheon, Korea South, Republic Of
J Kim, Pacific Northwest National Laboratory, Richland, Washington
S Kim, S Nair, Pennsylvania State University, University Park, Pennsylvania
J Lee, Chosun University, Gwangju, Korea South, Republic Of
D Lee, Korea Institute of Industrial Technology, Cheonan, Korea South, Republic Of

**Neuropeptides and Vasoactive Protein Detection from Human Skin**
CT Minson, University of Oregon, Eugene, Oregon

**New Theoretical Developments and Computational Studies of Complex Processes in Environmental Chemistry, Waste Containment, and Biochemistry**
K Burke, Rutgers University, Piscataway, New Jersey

AE Clark, Washington State University, Pulman, Washington
MC Wander, University of California, Davis, Davis, California
EJ Bylaska, R Devanathan, F Gao, Pacific Northwest National Laboratory, Richland, Washington
S Chumakov, Los Alamos National Laboratory, Los Alamos, New Mexico
N Marzari, HJ Kulik, N Bonini, B Kozinsky, NE Miller, T Thonhauser, Massachusetts Institute of Technology, Cambridge, Massachusetts
PA Moreira, Universidade Estadual De Campinas, Sao Paulo, Brazil
MV Losev, RA Evarestov, AI Panin, AV Bandura, St. Petersburg State University, St. Petersburg, Russian Federation
LR Corrales, JA Knibloe, University of Arizona, Tucson, Arizona
A Chartier, Commissariat a l\’Energie Nucleair, Gif-sur-Yvette, France
K Tsemekhman, Dn Baker, MA Gabriel, WR Schief, University of Washington, Seattle, Washington
J Du, University of North Texas, Denton, Texas
H Jonsson, University of Iceland, Reykjavík, Iceland
AV Morozov, The Rockefeller University, New York, New York
A Cormack

**Next Generation Clinical Proteomics to Target Human Health Challenges**
RD Smith, JM Jacobs, Pacific Northwest National Laboratory, Richland, Washington
MG Katze, University of Washington, Seattle, Washington

**NMR and Computational Studies of Chemical Transformations at Complex Interfaces**
E Iglesia, A Bhan, B Temel, University of California, Berkeley, Berkeley, California
J Hu, CH Peden, J Kwak, Y Wang, Pacific Northwest National Laboratory, Richland, Washington
DA Dixon, R Craciun, S Li, M Hernandez Matus, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
H Zheng, Dalian Institute of Chemical Physics, CAS, Dalian, China

**NMR and EPR Structural Characterization of c-Type Cytochromes and their Complexes from Contaminant Metal Remediating Iron-Respiring Bacteria**
TS Magnuson, Idaho State University, Pocatello, Idaho
JR Cort, Pacific Northwest National Laboratory, Richland, Washington

**NMR for Catalyst Studies**
CH Peden, Jn Hu, Y Wang, J Kwak, J Szanyi, Pacific Northwest National Laboratory, Richland, Washington

**NMR Studies of $^{207}$Pb in Ferroelectric Powders**
D Budker, AO Sushkov, LS Bouchard, C Qian, University of California, Berkeley, Berkeley, California

**NMR Studies of Li-Doped Wide Band $SnO_2$ Nanoparticles**
A Chaparadza, SB Rananavare, Portland State University, Portland, Oregon

**NMR Study of Ion Transport in Nanostructured Materials**
J Liu, Pacific Northwest National Laboratory, Richland, Washington

**NMR Study of Novel Hydrogen Storage Materials**

LL Shaw, University of Connecticut, Storrs, Connecticut
Z Yang, J Hu, V Murugesan, J Kwak, Pacific Northwest National Laboratory, Richland, Washington

**Non-Destructive Evaluation of Damaged Ancient Scrolls using NMR and Pixe Scanning to Separate Text from the Scroll Background Combined with 3D Virtual Unrolling**
WB Seales, RF Baumann, MD Field, University of Kentucky, Lexington, Kentucky
E Iuliano, Edward M. Iuliano, D.O., Richland, Washington

**Non-Empirical Simulations of Nuclear Fuel Materials**
P Van Uffelen, E Heifets, J Kotomins, D Grjaznovs, European Commission Joint Research Centre, Eggenstein-Leopoldshafen, Germany

**Non-Thermal Reactions in Thin Aqueous Films**
GA Kimmel, NG Petrik, Pacific Northwest National Laboratory, Richland, Washington
BO Olanrewaju, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia
MC Akin, University of Texas at Austin, Austin, Texas

**Non-Thermal Reactions in Thin Aqueous Films (Kay's BES-Surface Kinetics, PNNL Scope #16248)**
GA Kimmel, NG Petrik, Pacific Northwest National Laboratory, Richland, Washington
MC Akin, University of Texas at Austin, Austin, Texas

**Non-Thermal Reactions in Water Adsorbed on Anion-Doped $TiO_2$(110)**
GA Kimmel, NG Petrik, Pacific Northwest National Laboratory, Richland, Washington

**Novel Catalytic Materials for the Hydrodesulfurization and Water-Gas Shift Processes**
ME Bussell, AW Burns, AF Gaudette, Western Washington University, Bellingham, Washington

**NOx Adsorber Materials: Fundamental Studies, and Investigations of Sulfur Poisoning and Thermal Deactivation**
CH Peden, RS Disselkamp, D Kim, J Kwak, J Szanyi, RG Tonkyn, CM Verrier, D Tran, J Male, C Cao, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington

**Nucleation, Growth and Evaporation Rates of Aerosols**
SM Kathmann, CJ Mundy, Pacific Northwest National Laboratory, Richland, Washington
TL Windus, MS Gordon, EA Hull, LD Crosby, HM Netzloff, ND Atoms, Iowa State University, Ames, Iowa

**Observation of Biogenic Nano-scaled Wire-like Arsenic Sulfide Mineral**
JK Fredrickson, Pacific Northwest National Laboratory, Richland, Washington
J Lee, H Hur, Gwangju Institute of Science and Technology (GIST), Gwangju, Korea South, Republic Of

**OCD_Identification of Potential Plasma Biomarkers for Insulin Resistance Using Proteomics**
SM Varnum, J Pounds, Pacific Northwest National Laboratory, Richland, Washington

**On Improving Current Colloid Filtration Theory Models**
T Ginn, University of California, Davis, Davis, California
KE Nelson, Battelle Columbus, Davis, California

**Open Ocean Ship-Board Study of Atmospheric Aerosols at the Equatorial Pacific: Characterizing Iron in Marine Aerosol**
Y Dessiaterik, Colorado State University, Fort Collins, Colorado
V Shutthanandan, C Wang, Z Zhu, A Laskin, EMSL, Richland, Washington
AM Johansen, LS Shank, Central Washington University, Ellensburg, Washington
JW Murray, University of Washington, Seattle, Washington

**Orientation Studies of Lead Magnesium Niobate - Lead Titanate (PMN-PT) Single Crystal by X-Rays**
R Dhar, KG Lynn, MR Thurber, Washington State University, Pullman, Washington

**Oxide Clusters - Electronic Structure and Chemical Bonding Using Photoelectron Spectroscopy**
H Zhai, Washington State University, Richland, Washington
S Li, Xinzhou Teachers University, Xinzhou City, Shanxi, China
L Wang, Washington State University Tri-Cities, Richland, Washington

**Oxide Surface Structure and Acidity**
KM Rosso, SN Kerisit, Pacific Northwest National Laboratory, Richland, Washington
BR Bickmore, Brigham Young University, Provo, Utah
DM Smith, Whitman College, Walla Walla, Washington

**Oxygen Isotope Fractionation in Phosphate during Iron Oxide-Phosphate Interaction**
DP Jaisi, RE Blake, Yale University, New Haven, Connecticut

**Parameterization of Subsurface Flow and Transport Models for Multi-Scale Simulation**
ML Rockhold, M Oostrom, Pacific Northwest National Laboratory, Richland, Washington

**Pathogen Strain Detection Based on Changes in Expressed Proteins**
A Fox, University of South Carolina School of Medicine, Columbia, South Carolina

**Pathways and Fate of Individual Nanoparticles *in vivo*; a Whole Organism Approach**
R Tanguay, Oregon State University, Corvallis, Oregon
KJ Cassens, G Orr, Pacific Northwest National Laboratory, Richland, Washington

**PDSI Novel Scalability Research**
EJ Felix, EMSL, Richland, Washington

**Peptide Biomarker Analysis**
DS Wunschel, Pacific Northwest National Laboratory, Richland, Washington

**Phosphoproteome Determination of LPA Treated Osteocytes**
NJ Karin, Pacific Northwest National Laboratory, Richland, Washington

**Photochemical Processing of Organic Aerosol Particles Studied with High-Resolution Mass Spectrometry**
S Nizkorodov, AP Bateman, ML Walser, University of California, Irvine, Irvine, California
Y Dessiaterik, Colorado State University, Fort Collins, Colorado
A Laskin, EMSL, Richland, Washington

**Photochemical Studies on N-Doped $TiO_2$ Single Crystals - Fundamental Investigations of Water Splitting on Model $TiO_2$ (Mike Henderson's BES Project - 48526)**
VH Lam, University of Central Florida, Orlando, Florida
MA Henderson, SA Chambers, S Cheung, T Ohsawa, Z Dohnalek, Pacific Northwest National Laboratory, Richland, Washington
I Lyubinetsky, T Thevuthasan, P Nachimuthu, Y Du, EMSL, Richland, Washington
MK Bowman, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
R Shao, SC Andrews, unknown, Washington
Y Wang, Northwestern Polytechnical University, Xi'an, Shaanxi, China

**Photodesorption of Organic Radicals from $TiO_2$(110)**
A Wodtke, C Zhou, Y Ji, University of California, Santa Barbara, Santa Barbara, California
MA Henderson, Pacific Northwest National Laboratory, Richland, Washington
X Yang, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

**Photoluminescence of the Transition Metal-Oxygen Charge Transfer Absorption Band of Yttrium Aluminum Garnet**
CR Shawley, KG Lynn, Washington State University, Pullman, Washington

**Photoswitchable Dyes and Nanoparticles Enable High Resolution and Accurate Fluorescent Probes for Cell Imaging**
AD Li, Washington State University, Pullman, Washington
D Hu, Pacific Northwest National Laboratory, Richland, Washington

**Physicochemical Determinants of Distribution and Fate of Nanoparticles Following *in vivo* Exposure**
D Dutta, University of Florida, Gainesville, Florida
J Pounds, T Weber, KJ Cassens, J Teeguarden, G Orr, Pacific Northwest National Laboratory, Richland, Washington

**Pilot Study on Examination of LIRKO Islets and Serum Using Quantitative Proteomic Approaches**
W Qian, V Petyuk, Pacific Northwest National Laboratory, Richland, Washington
RN Kulkarni, Joslin Diabetes Center, Boston, Massachusetts

**Pipeline to High Performance**
AL Corrigan, Pacific Northwest National Laboratory, Richland, Washington
DE Cowley, D Wang, J Carr, EMSL, Richland, Washington

**pKa Measurements of Buried Carboxylic Side Chains in Reduced and Oxidized Forms of a Thioredoxin Homolog**
EJ Barbar, AR Hall, Oregon State University, Corvallis, Oregon

**Plan for Testing of the Acumen Plasma Emitter Array**
TA Blake, Pacific Northwest National Laboratory, Richland, Washington

RP Ginn, Acumen Scientific, Goleta, California
LM Fleenor, Sol Oriens, LLC, Albuquerque, New Mexico

**Platelet Proteome for Normal and Type-2 Diabetics**
DL Springer, Pacific Northwest National Laboratory, Richland, Washington

**Platelet Secretome**
RC Zangar, Pacific Northwest National Laboratory, Richland, Washington

**PNNL Metabolomics Measurement and Validation Development for Renewable Energy Research**
JC Scholten, J McLean, PD Majors, Pacific Northwest National Laboratory, Richland, Washington

**Preparation and Analysis of I-III-VI2 Nanomaterials for the Solar Energy Conversion and Radiation Sensing Applications**
JJ Pak, Ln Lau, JS Gardner, Idaho State University, Pocatello, Idaho

**Preparation of Stoichiometric $TiO_2$(110)-(1x1) Surface**
A Bondarchuk, H Freund, Fritz-Haber Institut der Max Planck Gesellschaft, Berlin, Germany

**Probing a Single Crystal Wide Gap Dilute Magnetic Semiconductor: Mn Doped Î$^2$-Ga$^2$O$_3$**
TC Lovejoy, MA Olmstead, F Ohuchi, University of Washington, Seattle, Washington

**Probing Dynamics within an Enzyme Family**
EZ Eisenmesser, JD Schlegel, University of Colorado at Denver, Aurora, Colorado

**Probing the Electronic Structures of Atomic Clusters and Solution Phase Species in the Gas Phase**
X Wang, J Yang, NS Parmar, X Xing, Washington State University, Richland, Washington
H Woo, The Scripps Research Institute, La Jolla, California
C Chi, Fudan University, Shanghai, China
S Li, Xinzhou Teachers University, Xinzhou City, Shanxi, China
L Wang, Washington State University Tri-Cities, Richland, Washington
G Xiao, Xi'an Jiaotong University, Xi'an, Shaanxi, China

**Product Analysis of Reactions of a Model System for Organics on Atmospheric Particles: Ozonolysis of Self-Assembled Monolayers on Silicon Surfaces**
TM McIntire, University of California, Irvine, Irvine, California

**Propane Reforming Process Development**
J Hu, DR Palo, RA Dagle, B Roberts, Pacific Northwest National Laboratory, Richland, Washington

**Prophylactic Cancer Vaccine**
T Liu, Pacific Northwest National Laboratory, Richland, Washington

**Proposal for Development of AMT Tag Database for *Clostridium themocellum* in Collaboration with Pacific Northwest National Laboratory**
D Wu, University of Rochester, Rochester, New York

**Protein Adsorption at the Metal Oxide/Water Interface by Second Harmonic Generation**
CM Eggleston, University of Wyoming, Laramie, Wyoming
L Shi, AG Joly, Pacific Northwest National Laboratory, Richland, Washington
J Boily, Umea University, Umea, Sweden

**Protein Complex Identification Using Novel Affinity Resins**
MU Mayer-Cumblidge, L Shi, TC Squier, P Yan, Pacific Northwest National Laboratory, Richland, Washington
S Verma. unknown, Washington

**Protein Complexes Altered by Oxidative Stress and Determined by FTICR-MS**
HS Smallwood, Pacific Northwest National Laboratory, Richland, Washington

**Protein Interactions and Interfaces**
G Montelione, Rutgers University, New Brunswick, New Jersey
MA Kennedy, TA Ramelot, Miami University, Oxford, Ohio
A Yee, University of Toronto (Univ. Health Network), Toronto, Ontario, Canada
JR Cort, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington
C Arrowsmith. University of Toronto, Toronto, Ontario, Canada

**Protein Structure and Surface Interactions of an Enamel Protein**
DL Masica, Johns Hopkins University, Baltimore, Maryland
GW Buchko, WJ Shaw, Pacific Northwest National Laboratory, Richland, Washington

**Proteome Investigations to Enable DOE Office of Biomass Programs Goals**
EA Panisko, Pacific Northwest National Laboratory, Richland, Washington

**Proteomic Analysis of Differential Growth in *Desulfovibrio spp.* for a Systems Biology Level Investigation**
JD Wall, DA Elias, BJ Giles, University of Missouri, Columbia, Columbia, Missouri

**Proteomic Analysis of Extracellular Appendages Displayed in *Desulfovibrio vulgaris***
DA Elias, University of Missouri, Columbia, Columbia, Missouri
YA Gorby, J. Craig Venter Institute, La Jolla, California

**Proteomic-Based Mechanistic Analysis of Components Involved in the Immunoprotective Pathways Regulated by Low-Dose Radiation and the Medicinal Mushroom *Trametes versicolor***
CA Sacksteder, Pacific Northwest National Laboratory, Richland, Washington
CA Wenner, M Martzen, Bastyr University, Kenmore, Washington

**Proteomic Characterization of *in vivo* and *in vitro* Model Systems of Hepatitis C Virus Infection: Global Quantitative Proteome AMT Tag Measurements of Cellular Protein Expression**
JM Jacobs, Pacific Northwest National Laboratory, Richland, Washington
MG Katze, DL Diamond, University of Washington, Seattle, Washington

**Proteomic Studies of Inflammation and the Host Response to Injury**
LL Moldawer, University of Florida, Gainesville, Florida

W Qian, T Liu, Pacific Northwest National Laboratory, Richland, Washington

**Proteomic Studies of Inflammation and the Host Response to Injury**
LL Moldawer, University of Florida, Gainesville, Florida
W Qian, BO Petritis, Pacific Northwest National Laboratory, Richland, Washington

**Proteomics Methods and QSAR models to Predict Nanoparticle Surface Chemistry Interactions**
T Liu, Pacific Northwest National Laboratory, Richland, Washington

**Proteomics of Populus: Understanding Protein Expression Involved in Carbon Allocation**
JD Johnson, Washington State University, Puyallup, Washington

**PTR-ITMS: Next Generation Aircraft Instrumentation (Alexander's ASP, PNNL Scope #47789)**
SP Garland, University of California, Davis, Redding, California
R Zaveri, CM Berkowitz, Pacific Northwest National Laboratory, Richland, Washington
MK Newburn, EMSL, Richland, Washington

**Pulsed EPR Studies of Nanocrystalline Zeolites and Hollow Zeolite Structures**
SC Larsen, University of Iowa, Iowa City, Iowa

**Pulsed Multiple Laser Deposition Facility for the Growth of Thin Films in Interfacial Combinatorial Material Exploration**
KM Beck, EMSL, Richland, Washington
F Ohuchi, E Venkatasubramanian, University of Washington, Seattle, Washington

**Purity Analysis of Synthetic Organic Compounds**
GW Buchko, S Harvey, B Wright, Pacific Northwest National Laboratory, Richland, Washington

**Quantification of the Ligand Effects in Transition Metal Coordination Compounds Using Electronic Structure Calculation Methods**
CA Tsipis, C Kefalidis, Aristotle University of Thessaloniki, Greece

**Quantitative Characterization of Protein Post-Translational Modifications Using Mass Spectrometry**
W Qian, S Ding, Q Zhang, T Heibeck, Pacific Northwest National Laboratory, Richland, Washington

**Quantitative Prediction of Kink Site Formation Rate on Calcite and Barite using Metadynamics**
JR Rustad, University of California, Davis, Davis, California
GK Schenter, SN Kerisit, Pacific Northwest National Laboratory, Richland, Washington
AG Stack, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia
SC Parker, University of Bath, Bath, United Kingdom

**Quorum Sensing in a Dissimilatory Metal Reducing Bacterium**
MF Hochella, DR Learman, Virginia Polytechnic Institute, Blacksburg, Virginia
BH Lower, The Ohio State University, Columbus, Ohio

**Radiation Induced Defects in Nanostructured Polymer-Derived Ceramics**
L An, University of Central Florida, Orlando, Florida

**Raman Capability for EMSL Users**
NJ Hess, Pacific Northwest National Laboratory, Richland, Washington

**Real-Time FTIR Measurements of Fe-Oxide Transformation in Presence of Dissimilatory Fe-Reducing Bacteria**
GG Geesey, Montana State University, Bozeman, Montana
TC Droubay, Pacific Northwest National Laboratory, Richland, Washington

**Real-Time Imaging of Lignocellulosic Biomass Degradation by Fluorescence Microscopy and Atomic Force Microscopy**
D Hu, Z Dai, KR Minard, L Wang, ZC Zhang, Pacific Northwest National Laboratory, Richland, Washington

**Real Time Study of Phase Transformation of $In_2Se_3$ Thin Films by PEEM**
F Ohuchi, MA Olmstead, C Lu, E Yitamben, University of Washington, Seattle, Washington

**Reduction of Technetium by Fe(II) Associated with Reduced Clay Mineral Nontronite**
H Dong, ME Bishop, Miami University, Oxford, Ohio
R Kukkadapu, EMSL, Richland, Washington

**Reduction of $U^{6+}$ by Magnetite and the Rate of Electron Transfer**
SN Kerisit, FN Skomurski, KM Rosso, Pacific Northwest National Laboratory, Richland, Washington
RC Ewing, U Becker, University of Michigan, Ann Arbor, Michigan

**Reductive Transformation of Iron Oxides: Coupled Solution and Solid-State Pathways**
GV Gibbs, Virginia Polytechnic Institute, Blacksburg, Virginia
KM Rosso, S Yanina, SN Kerisit, D McCready, TC Droubay, P Zarzycki, Pacific Northwest National Laboratory, Richland, Washington
P Meakin, Idaho National Engineering and Environmental Laboratory (INEEL), Idaho Falls, Idaho
C Wang, MH Engelhard, B Arey, EMSL, Richland, Washington

**Reforming of Hydrocarbons on Solid Oxide Fuel Cell Anodes**
Y Yang, A Karim, JJ Strohm, DL King, Y Wang, Pacific Northwest National Laboratory, Richland, Washington
X Wang, New Jersey Institute of Technology, Newark, New Jersey

**Reliable Electronic Structure Prediction of Molecular Properties**
KA Peterson, T Ichiye, Washington State University, Washington, Wash DC
C Ng, University of California, Davis, Davis, California
HF Schaefer, MC Lind, JM Turney, NM Marshall, JB Ingels, LD Speakman, NJ Stibrich, University of Georgia, Athens, Georgia
SS Xantheas, J Li, GS Fanourgakis, CJ Mundy, S Yoo, Pacific Northwest National Laboratory, Richland, Washington
BP Hay, Oak Ridge National Laboratory, Oak Ridge, Tennessee

I Dabkowska, University of Gdansk, Gdansk, Poland
JC Werhahn, Technische Universitat Munchen, Garching, Germany
S Niu, Georgetown University, Washington, Wash DC
DA Dixon, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
AK Wilson, NJ DeYonker, University of North Texas, Denton, Texas
M Haranczyk, Lawrence Berkeley National Laboratory, Berkeley, California
RA Bachorz, Universitaet Karlsruhe, Karlsruhe, Germany
MS Gutowski, A Whiteside, Heriot-Watt University, Edinburgh, United Kingdom
S Iwata, Toyota Physical and Chemical Research Institute, Aichi, Japan
L Wang, Washington State University Tri-Cities, Richland, Washington

**Reliable Relativistic Quantum Chemistry Calculations for Molecules with Heavy Elements**
WA Goddard, V Bryantsev, California Institute of Technology, Pasadena, California
J Autschbach, MT Sterzel, BC Mort, MA Rudolph, Research Foundation University at Buffalo, Buffalo, New York
BE Bursten, JL Sonnenberg, T Yang, Ohio State University, Columbus, Ohio
AE Clark, C Qin, Washington State University, Pullman, Washington
C Zhan, University of Kentucky, Lexington, Kentucky
IA Infante, Universiteit Amsterdam, Amsterdam, Netherlands
Z Zhang, Stanford University, Stanford, California
J Li, MC Perkins, PJ Nichols, V Glezakou, Pacific Northwest National Laboratory, Richland, Washington
ER Batista, Los Alamos National Laboratory, Los Alamos, New Mexico
BP Hay, Oak Ridge National Laboratory, Oak Ridge, Tennessee
KE Gutowski, University of Notre Dame, South Bend, Indiana
ML Mckee, H Sayin, Auburn University, Auburn, Alabama
L Visscher, SJ Van Gisbergen, C Jacob, Vrijie Universiteit/Scientific Computing and Modelling, Amsterdam, Netherlands
KG Dyall, Schrodinger, Inc., Portland, Oregon
WA De Jong, N Govind, EMSL, Richland, Washington
TL Windus, GE Schoendorff, Iowa State University, Ames, Iowa
DA Dixon, R Craciun, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
AK Wilson, University of North Texas, Denton, Texas
SM Walker, University of Manitoba, Winnipeg, Quebec, Canada
A Yakovlev, Scientific Computing and Modeling N.V., Amsterdam, The Netherlands, Netherlands
H Joo, University of the pacific, Stockton, California
WC Ermler, University of Texas at San Antonio, San Antonio, Texas
LG De Macedo, Sao Paulo State University, Bauru, SP, Brazil
MJ Kullman, Wichita State University, Wichita, Kansas

**Response of Radiation Detector Materials to Ions**
BD Milbrath, Pacific Northwest National Laboratory, Richland, Washington
W Zhang, Peking University, Beijing, China

**Reversible Organic Derivatization of Silica: Development of New Methods for Creating Template Imprinted Surfaces**
JP Peters, RM Jorgensen, Central Washington University, Ellensburg, Washington

**Role of Surface and Interface on Transport Properties in Nanoscale Conducting Oxides**

X Zhou, JW Templeton, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington

**Roles for Membrane Receptors in Cellular Responses to External Cues; The Case of ErbB4 and Morphology Dynamics**
C Lai, The Scripps Research Institute, La Jolla, California
G Orr, DJ Panther, JL Phillips, Pacific Northwest National Laboratory, Richland, Washington
S Vicini, Georgetown University, Washington DC, Wash DC

**Routine $^1$H and $^{13}$C NMR Analysis of Functionalized Semiconductor and Metallic Nanoparticles Synthesized for Biodetection Studies**
C Dutton, Washington State University, Richland, Washington
MG Warner, AM Pierson, Pacific Northwest National Laboratory, Richland, Washington
AM Shearrow, University of South Florida, Tampa, Florida

**Rudy Luck's Proposal**
RL Luck, Michigan Technological University, Houghton, Michigan

**Run ScalaBLAST on Proteomics Datasets**
CS Oehmen, AD Norbeck, GA Anderson, Pacific Northwest National Laboratory, Richland, Washington
ER Vorpagel, EMSL, Richland, Washington

**ScalaBLAST to Reduce Protein Sequence Redundancy, Determine Similarity Among Species, and Enable Proteomics on Unsequenced Microbial Communities**
AD Norbeck, ME Monroe, GA Anderson, SO Purvine, CS Oehmen, Pacific Northwest National Laboratory, Richland, Washington

**Scaling Up for Large Metagenomic Computations with ScalaBLAST**
TP Straatsma, J Nieplocha, CS Oehmen, AL Corrigan, AR Shah, Pacific Northwest National Laboratory, Richland, Washington
HJ Sofia, Whitman College, Walla Walla, Washington
DJ Baxter, EMSL, Richland, Washington
P Zuber, Oregon Health Sciences University/Oregon Graduate Institute, Beaverton, Oregon
E Szeto, VM Markowitz, Lawrence Berkeley National Laboratory, Berkeley, California
P Hugenholtz, NC Kyrpides, Joint Genome Institute, Walnut Creek, California

**Scanning and Transmission Electron Microscopy of Grape Berry Shrivel**
BR Bondada, Washington State University, Richland, Washington

**Screening Protein Crystals for XRD Data Collection at Synchrotrons**
GW Buchko, Pacific Northwest National Laboratory, Richland, Washington
DH Juers, Whitman College, Walla Walla, Washington

**Seattle Structural Genomics Center for Infectious Diseases**
GW Buchko, Pacific Northwest National Laboratory, Richland, Washington
G Varani, University of Washington, Seattle, Washington

**Secondary Ion Mass Spectroscopy Study of Transitions Metals Doped ZnO Nanowires**

N Athavan, R Könenkamp, Portland State University, Portland, Oregon

**Secondary Organic Aerosol Formation from Nitrate Photochemistry**
BJ Finlayson-Pitts, M Ezell, Y Yu, University of California, Irvine, Irvine, California
A Zelenyuk, R Zaveri, J Yang, Pacific Northwest National Laboratory, Richland, Washington
L Alexander, EMSL, Richland, Washington

**Secretome Analysis of Environmental Nanoparticle Induced Biomarkers**
JM Jacobs, BD Thrall, LM Masiello, SM Varnum, Pacific Northwest National Laboratory, Richland, Washington

**Selective Heterogeneous Catalysis**
LS Fifield, JT Bays, Pacific Northwest National Laboratory, Richland, Washington

**Self-Assembly and Phase Transitions in Nanofibers and Liposomes**
MJ McCullagh, GC Schatz, S Tonzani, ND Winter, O Lee, Northwestern University, Evanston, Illinois

**Semi-Experimental Equilibrium Structures for Molecules of Biological Significance**
TA Blake, RL Sams, Pacific Northwest National Laboratory, Richland, Washington
NC Craig, Oberlin College, Oberlin, Ohio

**SGI Altix Allocation for Advanced Computing Technology Lab**
J Nieplocha, AS Lipton, EJ Bylaska, CL Rakowski, JA Fort, BJ Palmer, MD Williams, SS Xantheas, PA Medvick, M Ovtchinnikov, Y Fang, M Singhal, ML Stewart, SM Robinson, AM Tartakovsky, DG Chavarria, DH Bacon, VL Freedman, GS Fanourgakis, J Li, LL Nuffer, M Krishnan, A Marquez, CS Oehmen, PD Ellis, WA Perkins, TR Shippert, S Kabilan, T Fu, Hn Silva, DR Einstein, SJ Bohn, DP Chassin, C Scherrer, G Lin, DR Rector, KP Recknagle, Pacific Northwest National Laboratory, Richland, Washington
D Wang, EMSL, Richland, Washington
EA Butterworth, University of Washington, Seattle, Washington
Z Yang, University of Colorado Boulder, Boulder, Colorado

**Shew Strains**
MS Lipton, S Deng, Pacific Northwest National Laboratory, Richland, Washington

**Simultaneous Optical & Chemical Measurements of Aerosols as a Function of Relative Humidity: Bridging Laboratory and Field Measurements to Models**
MK Dubey, Los Alamos National Laboratory, Los Alamos, New Mexico

**Single Enzyme Nanoparticles**
P Wang, University of Minnesota, Minneapolis, Minnesota
J Kim, JW Grate, Pacific Northwest National Laboratory, Richland, Washington
H Na, Seoul National University, Seoul, Korea South, Republic Of
S Shin, H Park, H Chang, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea South, Republic Of
S Kim, Pennsylvania State University, University Park, Pennsylvania

**Single Molecule Studies of Multi-Chromophoric Foldamers**
AD Li, W Wu, Washington State University, Pullman, Washington
D Hu, Pacific Northwest National Laboratory, Richland, Washington

**Site-Specific Sample Preparation of Surfaces and Buried Interfaces for TEM and Atom Probe Analysis**
LE Thomas, M Olszta, Pacific Northwest National Laboratory, Richland, Washington
B Arey, EMSL, Richland, Washington

**Site-Specific Surface Excitation of Calcium Oxide "Nanocubes"**
O Diwald, Vienna University of Technology, Wien, Austria

**Soft-Landing of Complex Ions on Surfaces**
JR Green, RG Cooks, MP Goodwin. Purdue University, West Lafayette, Indiana
J Laskin, O Hadjar, P Wang, JH Futrell, AS Lea, Pacific Northwest National Laboratory, Richland, Washington
Z Zhu, PL Gassman, EMSL, Richland, Washington
Z Yang. University of Colorado Boulder, Boulder, Colorado
W Peng, National Dong Hwa University, Shoufeng, Hualien, Taiwan, Province Of China

**Solid State $^{11}$B-NMR Analysis of the Decomposition Products of Ammonia-Borane Thermolysis in Ionic Liquids for Hydrogen Storage**
LG Sneddon, LR Alden, DW Himmelberger, University of Pennsylvania, Philadelphia, Pennsylvania

**Solid-State NMR Characterization of Semiconductor Nanoparticle/Polymer Interfaces**
MP Espe, SY Ortiz, University of Akron, Akron, Ohio

**Solid-State NMR Spectroscopy on Radioactive Samples with Microcoils**
I Farnan, University of Cambridge, Cambridge, United Kingdom
D Sakellariou, CEA Saclay, Gif-sur-Yvette, France

**Solid-State NMR Structural Studies of HIV-1 CA Protein Assembly**
TE Polenova, Y Han, S Paramasivam, University of Delaware, Newark, Delaware

**Solution Structure of a 42 kDa "Metal Sensor" CzrA-DNA Complex**
AK Alphonse Ignatius, DP Giedroc, Indiana University - Bloomington, Bloomington, Indiana

**Soybean Proteomics**
G Stacey, University of Missouri, Columbia, Columbia, Missouri

**Spatially Resolved Proteomic studies of Brains Obtained from Control Mice and Treated Mice Simulating Parkinson's Disease**
W Qian, Pacific Northwest National Laboratory, Richland, Washington

**Specificity of *Shewanella oneidensis* Outer Membrane Cytochromes OmcA and OmcB Towards Iron- and Manganese-Oxide Surfaces**
TC Droubay, L Shi, Pacific Northwest National Laboratory, Richland, Washington
BH Lower, The Ohio State University, Columbus, Ohio

**Spectral Library (Sharpe's NNSA, PNNL Scope #28727)**
SW Sharpe, TA Blake, TJ Johnson, RL Sams, DC Scott, RG Tonkyn, Pacific Northwest National Laboratory, Richland, Washington

**Spectroelectrochemical Sensor for Pertechnetate, $TcO_4^-$, Applicable to Hanford and Other DOE Sites**
SA Bryan, WD Samuels, S Hightower, Pacific Northwest National Laboratory, Richland, Washington
WR Heineman, CJ Seliskar, University of Cincinnati, Cincinnati, Ohio

**Spectroscopic Investigation of Hg(II) reduction by Magnetite**
N Yee, Rutgers University, New Brunswick, New Jersey

**Spin Electronic Phenomena in Magnetically Doped Perovskites and Complex Oxide Interfaces**
TC Kaspar, SA Chambers, TC Droubay, Pacific Northwest National Laboratory, Richland, Washington
C Wang, V Shutthanandan, T Thevuthasan, MH Engelhard, EMSL, Richland, Washington

**Spin Valve with Perpendicular Anisotropy for Spin Torque Experiments**
A Pakhomov, K Krishnan, University of Washington, Seattle, Washington

**Stable Isotope Ratios of Cyanides and Phosgene**
HW Kreuzer, AJ Carman, Pacific Northwest National Laboratory, Richland, Washington
L Alexander, EMSL, Richland, Washington

**Stopping Power Measurements of Heavy Ions over a Wide Range of Energy**
R Linares, Universidade de Sao Paulo, Sao Paulo, Brazil
Y Zhang, EMSL, Richland, Washington

**Strontium in Inorganic Materials Studied with High-Field Solid-State NMR Spectroscopy**
KT Mueller, CR Strepka, MC Davis, Pennsylvania State University, University Park, Pennsylvania

**Structure and Catalytic Activity of Supported Early Transition Metal Oxide Clusters**
S Li, Tulane University, New Orleans, Louisiana
Z Dohnalek, BD Kay, Z Zhang, R Rousseau, Pacific Northwest National Laboratory, Richland, Washington
JM White, Y Kim, J Gong, University of Texas at Austin, Austin, Texas

**Structure and Dynamics of Ca in Clays, Mineral Phases of Concrete, and Ca-NOM Complexes: Natural Abundance Ca-43 NMR and Molecular Modeling Studies**
AG Kalinichev, RJ Kirkpatrick, GM Bowers, Michigan State University, East Lansing, Michigan

**Structure-Function Correlations of Proteins in Enamel Formation**
WJ Shaw, BJ Tarasevich, GW Buchko, AS Lea, Pacific Northwest National Laboratory, Richland, Washington
ML Snead, University of Southern California, Los Angeles, California

**Structure-Property Relationships in Thin Film Energy Conversion Materials and Coatings**
DW Matson, PE Burrows, LC Olsen, PM Martin, ME Gross, WD Bennett, CC Bonham, G Graff, ES Mast, SN Kundu, AB Padmaperuma, L Sapochak, AL Von Ruden,

PK Koech, H Qiao, J Ryan, Xn Cai, J Rainbolt, DJ Gaspar, Y Shin, J Swensen, AG Joly, SA Towne, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington

**Structural Analysis of Ion-Beam-Induced Amorphous SiC by Advanced Electron Microscopy**
M Ishimaru, A Hirata, M Naito, Y Hirotsu, Osaka University, Ibaraki, Japan

**Structural Criteria for the Design of Anion Receptors: The Interaction of Halides with Nitrogen-Containing Heterocyclic Compounds**
V Bryantsev, California Institute of Technology, Pasadena, California
BP Hay, Oak Ridge National Laboratory, Oak Ridge, Tennessee

**Structural Studies of a Family of Proteins from the Diurnal Cyanobacteria *Cyanothece* 51142 that Contain an Unusual Repeated Five-Residues Domain (RFR)**
S Ni, MA Kennedy, Miami University, Oxford, Ohio
GW Buchko, Pacific Northwest National Laboratory, Richland, Washington
HB Pakrasi, Washington University in St. Louis, St. Louis, Missouri

**Studies of Nanomaterials for Removal of Perchlorate in Water**
Y Lin, Z Tang, H Wang, J Wang, Pacific Northwest National Laboratory, Richland, Washington
X Kang, Guangdong Ocean University, Guangdong, China

**Studies on 1,2,3-Trichloropropane (TCP) and Its Derivatives**
EJ Bylaska, M Dupuis, Pacific Northwest National Laboratory, Richland, Washington
AR Felmy, M Valiev, EMSL, Richland, Washington
DA Dixon, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama
PG Tratnyek, Oregon Health Sciences University/Oregon Graduate Institute, Beaverton, Oregon

**Study of Interfacial Phenomena of Novel-Layered Thin Film Structure**
Y Zhang, EMSL, Richland, Washington
Y Liu, X Wang, Alfred University, Alfred, New York

**Study of the Initial Oxide Scale Formation and Growth on Haynes 214 Alloy at 800 & 900C**
P Singh, C Vasil, Pacific Northwest National Laboratory, Richland, Washington

**Study of Thermal Decomposition of Polyester Fibers Treated with Phosphorus Flame Retardants**
S Gaan, G Sun, University of California, Davis, Davis, California

**Structure and Bonding in Actinide Oxides**
SD Conradson, Los Alamos National Laboratory, Los Alamos, Afghanistan

**Structure and Recognition in Microbial Membranes Proteins, and DNA**
JH Miller, A Aceves-Gaona, MB Ernst, A Suleiman, Washington State University, Richland, Washington
MA Kennedy, Miami University, Oxford, Ohio
TP Straatsma, M Dupuis, LN Douali, RD Lins, TA Da Silva, J Harper, Pacific Northwest National Laboratory, Richland, Washington

MS Sansom, JP Armitage, JP Pikunic, KL Cox, S Khalid, Ln Vaccaro, University of Oxford, Oxford, United Kingdom
I Dabkowska, University of Gdansk, Gdansk, Poland
M Valiev, ER Vorpagel, EMSL, Richland, Washington
P Hobza, Academy of Sciences of the Czech Republic, Prague 6, Czech Republic
R Gabdoulline, University of Heidelberg, Heidelberg, Germany
M Haranczyk, Lawrence Berkeley National Laboratory, Berkeley, California
RA Bachorz, Universitaet Karlsruhe, Karlsruhe, Germany
MS Gutowski, A Whiteside, S Ling, Heriot-Watt University, Edinburgh, United Kingdom
MW Zacharias, F Sieker, Jacobs University Bremen, Bremen, Germany
BH Lower, The Ohio State University, Columbus, Ohio

**Structural Biology of the Human High Mobility Group A (HMGA) Proteins**
RC Reeves, K McAteer, Washington State University, Richland, Washington
MA Kennedy, Miami University, Oxford, Ohio
GW Buchko, Pacific Northwest National Laboratory, Richland, Washington

**Structure, Composition, and Phase Behavior of Mixed Biphenylthiol Self-Assembled Monolayers**
EL Bullock, Central Washington University, Ellensburg, Washington

**Structural Engineering of the *de novo* Designed Protein Top7 as a Scaffold for Antigen-Binding**
TP Straatsma, TA Da Silva, CL Baird, DO Apiyo, CB Boschek, Pacific Northwest National Laboratory, Richland, Washington

**Structural Investigation of Human Small Heat Shock Proteins Alpha-Beta-Crystallin and HSP27**
R Klevit, P Rajagopal, University of Washington, Seattle, Washington

**Structural Studies of Regulators of Histone Protein Synthesis**
R Thapar, University of North Carolina, Buffalo, New York

**Substrate-Specific Binding of *Staphylococcus adhesins* to Solid Surfaces**
S Lower, Z Oestreicher, Ohio State University, Columbus, Ohio
C Gassman, Columbia Basin College, Pasco, Washington
BH Lower, The Ohio State University, Columbus, Ohio

**Subsurface Reductive Elimination of Trichloroethylene using Zero-Valent Iron Emplaced by Polymer Solutions**
MJ Truex, M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**Subunit Structures of Arabidopsis RNA Polymerase IV complexes**
CS Pikaard, Washington University in St. Louis, Saint Louis, Missouri
L Pasa-Tolic, EMSL, Richland, Washington

**Surface and Bulk Characterization of Ambient Ultrafine Particles**
EL Bullock, AM Johansen, C Thomas-Bradley, JM Johnston, TK O'Connell, JK Wells, Central Washington University, Ellensburg, Washington

**Surface and Interface Studies of Photochemically Initiated Immobilization**
S Chada, M Yan, L Liu, DJ Henry, RR Bard, K Wang, Y Miao, SN Uppalapati, X Wang, Portland State University, Portland, Oregon
MH Engelhard, EMSL, Richland, Washington

**Surface Chemistry of Nanocrystalline Zeolites Probed by Magnetic Resonance Techniques**
WM Ames, SC Larsen, University of Iowa, Iowa City, Iowa
MK Bowman, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**Surface Migration of Additives in Polymers**
LA Archer, Z Qian, Cornell University, Ithaca, New York

**Surface Plasmon Polariton Dependence on Metal Surface Morphology**
RE Peale, University of Central Florida, Orlando, Florida
KM Beck, EMSL, Richland, Washington

**Surface Selective Studies of Olivine Dissolution by $^{1}$H-$^{29}$Si CP and $^{25}$Mg MQMAS NMR**
KT Mueller, MC Davis, WJ Brouwer, CR Strepka, DL Suchy, Pennsylvania State University, University Park, Pennsylvania

**Synthesis and Single-Crystal X-ray Characterization of Cluster-Assembled Materials**
Z Sun, Washington State University, Richland, Washington
L Wang, Washington State University Tri-Cities, Richland, Washington

**Synthesis of Highly Uniform Magnetic Nanoparticles with Enhanced Moment Density**
J Yang, X Gao, University of Washington, Seattle, Washington

**Synthesis of Nanostructured Materials and Cluster-Assembled Materials**
Z Sun, Washington State University, Richland, Washington
MH Engelhard, EMSL, Richland, Washington
L Wang, Washington State University Tri-Cities, Richland, Washington

**Synthesis of Photoactive Metal Oxide Films for Study Using Time-Resolved X-Ray Techniques**
PB Hillyard, Stanford University, Stanford, California
KJ Gaffney, JR Bargar, Stanford Synchrotron Radiation Laboratory, Menlo Park, California

**Systems Biology of Iron, Carbon, and NitrogenMetabolism in the Marine Diatom *Phaeodactylum tricornutum***
AE Allen, J. Craig Venter Institute, San Diego, California

**TEM Study of Interfacial Layers in Nb-Clad Stainless Steel**
I Bae, J Choi, KS Weil, Pacific Northwest National Laboratory, Richland, Washington

**TEM Study on SOFC Interconnects and Interfaces**
Z Yang, Pacific Northwest National Laboratory, Richland, Washington

**Temperature Dependent High-Resolution UV- and IR-Absorption-Cross-Section Spectra of Low-Volatility SOA Precursor Hydrocarbons in the Gas-Phase**

TJ Johnson, Pacific Northwest National Laboratory, Richland, Washington
RM Volkamer, MJ Molina, University of California, San Diego, La Jolla, California

**Terrestrial Carbon Sequestration Studies**
JE Amonette, Pacific Northwest National Laboratory, Richland, Washington

**Test Measurements and Approaches for Enhancing Information Available from Surface Analysis of Oxides, Nanoparticles and Organic Materials Analysis**
DR Baer, MH Engelhard, EMSL, Richland, Washington
DG Castner, SD Techane, University of Washington, Seattle, Washington
R Wallace, University of Texas at Dallas, Richardson, Texas
S Suzer, Bilkent University, Ankara, Turkey

**The Aerosol Modeling Testbed**
JD Fast, WI Gustafson, EG Chapman, Pacific Northwest National Laboratory, Richland, Washington
DJ Baxter, EMSL, Richland, Washington

**The Binding Energetics of Methane on Water Ice Surfaces**
RS Smith, BD Kay, Pacific Northwest National Laboratory, Richland, Washington
CD Neish, University of Arizona, Tucson, Arizona

**The Characterization of Adsorbed Fe(II) And Its Reactivity with Nitrite**
CJ Matocha, University of Kentucky, Lexington, Kentucky
R Kukkadapu, EMSL, Richland, Washington

**The Characterization of Diesel Exhaust Particle Matter and its Atmospheric Lifecycle: The Size, Shape and Composition of Soot Particles in the Atmosphere**
GG Muntean, GD Maupin, A Zelenyuk, J Yang, Pacific Northwest National Laboratory, Richland, Washington

**The Cloud Nucleating Properties of Aerosols at a Continental Site: CHAPS Study**
JN Olfert, Brookhaven National Laboratory, Upton, New York
Y Dessiaterik, Colorado State University, Fort Collins, Colorado
A Laskin, EMSL, Richland, Washington
MK Gilles, Lawrence Berkeley National Laboratory, Berkeley, California
J Wang, Shenyang Pharmaceutical University, Shenyang, China

**The Effect of Surface Active Organic Molecules on the Water Uptake, Shape and Density of Hygroscopic Particles of Atmospheric Importance**
GB Ellison, LA Cuadra-Rodriguez, University of Colorado, Boulder, Colorado
A Zelenyuk, J Yang, Pacific Northwest National Laboratory, Richland, Washington

**The Effects of Gamma-Irradiation on the Fe(II)/Fe(III) Signatures in Iron Oxide and Iron Silicate Minerals**
TL Bank, Research Foundation University at Buffalo, Buffalo, New York

**The Electronic Structure and Dynamics of Photocatalytic and Electronic Interfaces**
J Zhao, H Petek, University of Pittsburgh, Pittsburgh, Pennsylvania

**The Formation and Structure of Tropical Organic/Water Aerosols**
GB Ellison, LA Cuadra-Rodriguez, University of Colorado, Boulder, Colorado

A Zelenyuk, R Zaveri, J Yang, Pacific Northwest National Laboratory, Richland, Washington
Y Dessiaterik, Colorado State University, Fort Collins, Colorado
A Laskin, EMSL, Richland, Washington

**The Impact of Carbonate on Surface Protonation, Electron Transfer and Crystallization Reactions in Iron Oxide Nanoparticles and Colloids**
JR Rustad, University of California, Davis, Davis, California
J Boily, Umea University, Umea, Sweden
DA Dixon, M Hernandez Matus, MT Nguyen, VE Jackson, University of Alabama, Tuscaloosa, Tuscaloosa, Alabama

**The *in vivo* Localization and Interactions between Structural Components of the *Shewanella oneidensis* MR-1 Metal Reducing System by High Resolution Transmission Electron Microscopy**
GG Geesey, Montana State University, Bozeman, Montana
MJ Marshall, Pacific Northwest National Laboratory, Richland, Washington
A Dohnalkova, EMSL, Richland, Washington

**The Interaction of HCl on Water Ice Nanoscale Films**
RS Smith, BD Kay, Pacific Northwest National Laboratory, Richland, Washington
P Ayotte, Universite de Sherbrooke/Concordia University (University of Sherbrooke), Sherbrooke, Quebec, Canada

**The Iron Binding Environment of the Cyanobacterial Ferric Ion Transporter, FutA1**
TJ Smith, Donald Danforth Plant Science Center, Saint Louis, Missouri

**The Oxidation of Self Assembled Organic Monolayers by Nitrate Radicals using Time of Flight Secondary Ion Mass Spectrometry**
AK Bertram, University of British Columbia, Vancouver, British Columbia, Canada

**The Reduction of Uranyl and Chromate to Insoluble Species by Green Rust and Other Ferrous Hydroxides Surfaces**
MC Wander, University of California, Davis, Davis, California
KM Rosso, Pacific Northwest National Laboratory, Richland, Washington
MA Schoonen, State University of New York at Stony Brook, Stony Brook, New York

**The Relationship between Particle Properties and Ice Nucleation: Laboratory and Field Investigation and Parameterization Development**
X Liu, A Zelenyuk, SJ Ghan, J Yang, Pacific Northwest National Laboratory, Richland, Washington

**The Role of Extracellular Polymeric Substances in Bacterial Fouling of Membranes**
KM Rosso, Pacific Northwest National Laboratory, Richland, Washington
B Korpol, S Chellam, AR Badireddy, University of Houston, Houston, Texas

**The Role of Ice and Aerosol Surfaces in Halogen Activation in the Arctic Springtime Boundary Layer**
Y Dessiaterik, Colorado State University, Fort Collins, Colorado
WR Simpson, DM Carlson, University of Alaska, Fairbanks, Fairbanks, Alaska
A Laskin, V Shutthanandan, EMSL, Richland, Washington
L Alvarez-Aviles, University of Alaska Fairbanks, Fairbanks, Alaska

**The Role of PdZn Alloy Formation and Particle Size on the Selectivity for Steam Reforming of Methanol**
VM Lebarbier, Pacific Northwest National Laboratory, Richland, Washington
AM Karim, A Datye, TR Conant, University of New Mexico, Albuquerque, New Mexico

**The Role of U(V) during Heterogeneous Reduction of Aqueous U(VI) to U(IV)**
ES Ilton, Pacific Northwest National Laboratory, Richland, Washington
MH Engelhard, EMSL, Richland, Washington
J Boily, Umea University, Umea, Sweden

**The Study of Atomic Gold Clusters in Polyaniline**
AH Saheb, M Josowicz, JA Janata, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia

**The Unoccupied Electronic Structure of Surface Adsorbates**
H Petek, J Zhao, University of Pittsburgh, Pittsburgh, Pennsylvania

**Theoretical Investigations of Chiral Self-Assembly at Solid Surfaces**
M Ratner, Northwestern University, Evanston, Illinois
I Paci, University of Victoria, Victoria, British Columbia, Canada

**Thermodynamic and Chemical Properties of La1-xSrxCoxFe1-xO3 from First-Principles Calculations: Implications for Use as SOFC Cathodes**
SB Sinnott, C Lee, University of Florida, Gainesville, Florida

**Thin Film Electrolyte/Electrode Development and Enhanced Ionic Transport in Miniaturized Solid Oxide Fuel Cells on Silicon Chips**
P Singh, O Marina, Pacific Northwest National Laboratory, Richland, Washington

**Three-Dimensional Structural Analysis of Altered Micas by Ion Beam/Scanning Electron Microscopy (FIB/SEM Dual Beam), μ-X-ray Diffraction, and Transmission Electron Microscopy**
J Mckinley, Pacific Northwest National Laboratory, Richland, Washington
B Arey, P Nachimuthu, EMSL, Richland, Washington

**Thrust Area 1: Characterization of Purified Proteins for Distribution to Grand Challenge Participants (EMSL User Support)**
L Shi, Pacific Northwest National Laboratory, Richland, Washington

**Thrust Area #2: Molecular Modeling of Electron Transfer in Fe(III) Oxides**
MC Wander, University of California, Davis, Davis, California
KM Rosso, SN Kerisit, FN Skomurski, X Wang, Pacific Northwest National Laboratory, Richland, Washington
DM Smith, Whitman College, Walla Walla, Washington
M Valiev, EMSL, Richland, Washington
JD Kubicki, Pennsylvania State University, University Park, Pennsylvania

**Thrust Area 3: Mutagenesis and Functional Characterization of *Shewanella oneidensis* Genes Involved in Fe(III) and Mn(IV) Oxide Reduction (LDRD #3)**
TJ Beveridge, University of Guelph, Guelph, Ontario, Canada

AS Beliaev, MF Romine, JK Fredrickson, Pacific Northwest National Laboratory, Richland, Washington
T Dichristina, Georgia Institute of Technology, Georgia Tech Research Corporation, Atlanta, Georgia
TW Wietsma, EMSL, Richland, Washington

**Thrust Area 4: How Redox Proteins on the Exterior of the Outer Membrane of *Shewanella* Accomplish Interfacial Electron Transfer to the Fe(III) Oxide Surface**
CM Eggleston, University of Wyoming, Laramie, Wyoming
AM Spormann, J Ha, Stanford University, Stanford, California
TC Droubay, Pacific Northwest National Laboratory, Richland, Washington

**Thrust 4: Model Hematite Thin Films and Bacterial Iron Reduction (LDRD: Cytochrome and Whole Cell Interactions with Iron Oxides)**
TC Droubay, Z Wang, L Shi, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington
BH Lower, The Ohio State University, Columbus, Ohio

**Thrust 4: Whole Cell and Cytochrome Biological Force Microscopy (LDRD: Cytochrome and Whole Cell Interactions with Iron Oxides)**
BH Lower, The Ohio State University, Columbus, Ohio

**Time-Resolved Study of Phase Transformation of $In_2Se_3$ Thin Films by PEEM**
KM Beck, EMSL, Richland, Washington
F Ohuchi, MA Olmstead, C Lu, E Yitamben, University of Washington, Seattle, Washington

**Tissue Distribution and Fate of Nanoparticles Following *in vivo* Exposure**
G Orr, Pacific Northwest National Laboratory, Richland, Washington
K Sarlo, The Procter and Gamble Company, Fairfield, Ohio

**Todd Allen's Proposal**
TR Allen, L Tan, AM Kruizenga, University of Wisconsin-Madison, Madison, Wisconsin

**Toward Preparation and *operando* Characterization of Nanostructured Heterogeneous Photocatalysts**
Y Shin, GE Fryxell, XS Li, RE Williford, K Parker, Pacific Northwest National Laboratory, Richland, Washington

**Transparent Circuits**
F Hua, Clarkson University, Potsdam, New York

**Trauma & Sepsis Induced Changes in Immune Cell Membrane Receptor Trafficking**
J Cuschieri, University of Washington, Seattle, Washington

**Trauma-Induced Reprogramming: Changes in Lipid Raft Protein Content**
V Petyuk, Pacific Northwest National Laboratory, Richland, Washington
J Cuschieri, University of Washington, Seattle, Washington

**Tuning the Chemistry and Configuration of Oxide Nanostructures for Energy and Environmental Applications**
S Seal, AS Karakoti, University of Central Florida, Orlando, Florida

**Ultrafast Laser Interactions with Wide Bandgap Materials**
JT Dickinson, E Khan, Washington State University, Pullman, Washington
WP Hess, AG Joly, Pacific Northwest National Laboratory, Richland, Washington

**Ultrahigh-Field $^{95}$Mo MAS NMR Studies of Model Nuclear Waste Glasses**
I Farnan, University of Cambridge, Cambridge, United Kingdom
S Kroeker, University of Manitoba, Winnipeg, Manitoba, Canada

**Ultrastructure of Aerial Interface in Apple**
EA Curry, USDA, ARS, Tree Fruit Research Laboratory, Wenatchee, Washington

**Understanding and Development of Novel NanoMaterials for Frequency Upconversion**
K Yu, National Research Council of Canada, Ottawa, Ontario, Canada
W Chen, University of Texas at Arlington, Arlington, Texas

**Understanding Field-Dependent Quadrupolar Splitting of $^{131}$Xe for Applications to Surface/Material Studies**
KF Stupic, T Meersmann, Colorado State University, Fort Collins, Colorado

**Understanding Microorganism-Metal Interactions**
BE Kimball, SL Brantley, Pennsylvania State University, University Park, Pennsylvania

**Understanding of Long-Term Phase Stability and Degradations in Solid Oxide Fuel Cells**
P Singh, DL King, LR Pederson, Pacific Northwest National Laboratory, Richland, Washington
N Govindaraju, University of Cincinnati, Cincinnati, Ohio
L Miara, Boston University, Brookline, Massachusetts

**Understanding the Influence of Radiation Exposure on Ceria Nanoparticle Surface Chemistry**
S Seal, University of Central Florida, Orlando, Florida

**Understanding the Mechanisms and Enhancement of Photostimulated Luminescence by Nanoscale Design and Fabrication**
W Chen, University of Texas at Arlington, Arlington, Texas

**Understanding the Structure-Catalytic Function Relationship of Cobalt Based Catalysts for Steam Reforming of Ethanol**
SY Ha, Washington State University, Pullman, Washington

**Understanding the Structure-Catalytic Function Relationship of Cobalt Based Catalysts for Steam Reforming of Oxygenated Hydrocarbons**
SY Ha, S Lin, Washington State University, Pullman, Washington

**Undoped and n-Type Doped $TiO_2$ Anatase Surface Structures and Reactivity with Water**
S Chamberlin, University of Wisconsin, Milwaukee, Wisconsin
CJ Hirschmugl, University of Wisconsin, Milwaukee, MIlwaukee, Wisconsin

**Use of Inductively Coupled Plasma Atomic Emission Spectrometer for Determining Metal Ion Uptake by New Extraction Chromatography or Ion Exchange Resins**
GJ Lumetta, Pacific Northwest National Laboratory, Richland, Washington

**Use of Wet Chemical Facilities in the EMSL 1310 Laboratory - Protein Pipeline (Marvin Warner's DHS Project - 47443)**
C Dutton, Washington State University, Richland, Washington
MG Warner, AM Pierson, Pacific Northwest National Laboratory, Richland, Washington
AJ Tyler, Utah State University, Logan, Utah

**Using Metallic Interlayers to Stabilize Metal-Metal Interface**s
RJ Smith, WA Priyantha, A Comouth, H Chen, Montana State University, Bozeman, Montana

**V-51 Solid-State NMR and Density Functional Theory Studies of Vanadium Haloperoxidases**
TE Polenova, S Bolte, S Sun, S Paramasivam, University of Delaware, Newark, Delaware

**Validation of Whole-Core Determination of Soil Hydraulic Properties**
MJ Fayer, Pacific Northwest National Laboratory, Richland, Washington

**Variable-Temperature Mössbauer Spectroscopy of Aluminum-Substituted Maghemites**
MA Batista, Ohio State University, Columbus, Ohio
JM Bigham, The Ohio State University, Columbus, Ohio

**Visualization of a Pd-Au{100} Catalyst: A Scanning Tunneling Microscopy Study**
P Han, DW Goodman, F Yang, Texas A&M University, College Station, Texas

**Visualization of a Pt-Co(111) Catalyst: A Scanning Tunneling Microscopy Study**
F Yang, DW Goodman, Texas A&M University, College Station, Texas

**Visualization of Soot-Trapped Diesel Particulate Filters (DPF) using Nuclear Magnetic Resonance Imaging**
J Kwak, D Kim, CH Peden, Pacific Northwest National Laboratory, Richland, Washington

**WaNPRC Macaque Proteomics for Models of Influenza Infection and AIDS**
DG Camp, Pacific Northwest National Laboratory, Richland, Washington

**Wettability and Mass Transfer Effects on Flow and Transport of Mixed DNAPL in Hanford Site Sediments**
C Werth, AJ Valocchi, University of Illinois, Urbana-Champaign, Illinois
M Oostrom, MA Covert, Pacific Northwest National Laboratory, Richland, Washington
TW Wietsma, EMSL, Richland, Washington

**WRI Breast Cancer**
KD Rodland, DG Camp, T Liu, Pacific Northwest National Laboratory, Richland, Washington
RJ Mural, Windber Research Institute, Windber, Pennsylvania

**XRD of CsI Scintillators**
K Krishnaswami, B Cannon, Pacific Northwest National Laboratory, Richland, Washington

# Fiscal Year 2008 Publications

Publications by EMSL staff members and from users where the publication resulted from research carried out at EMSL are listed below.

**Journal Articles**

Alejandro PBG, S Zhu, K Sun, X Xiang, Y Zhang, and LM Wang. 2008. "Embedded Nanofibers Induced by High-Energy Ion Irradiation of Bulk GaSb." *Small* 4(8):1119-1124. doi:10.1002/smll.200701236

Ansong CK, H Yoon, AD Norbeck, JK Gustin, JE McDermott, HM Mottaz, J Rue, JN Adkins, F Heffron, and RD Smith. 2008. "Proteomics Analysis of the Causative Agent of Typhoid Fever." *Journal of Proteome Research* 7(2):546-557. doi:10.1021/pr070434u

Ansong CK, SO Purvine, JN Adkins, MS Lipton, and RD Smith. 2008. "Proteogenomics: Needs and Roles to be Filled by Proteomics in Genome Annotation." *Briefings in Functional Genomics and Proteomics* 7(1):50-62. doi:10.1093/bfgp/eln010

Averkiev BB, AI Boldyrev, X Li, and LS Wang. 2007. "Planar Nitrogen-Doped Aluminum Clusters AIxN- (x=3-5)." *Journal of Chemical Physics* 125(12): Art. No. 124305. doi:10.1063/1.2335449

Averkiev BB, S Call, AI Boldyrev, L Wang, W Huang, and LS Wang. 2008. "Photoelectron Spectroscopy and Ab Initio Study of the Structure and Bonding in $A^{17}$N- and $A^{17}$N." *Journal of Physical Chemistry A* 112(09):1873-1879. doi:10.1021/jp7106236 S1089-5639(71)00623-6

Averkiev BB, DY Zubarev, LM Wang, W Huang, LS Wang, and AI Boldyrev. 2008. "Carbon Avoids Hypercoordination in CB6-, CB62-, and C2B5- Planar Carbon-Boron Clusters." *Journal of the American Chemical Society* 130(29):9248-9250. doi:10.1021/ja801211p

Badireddy AR, S Chellam, S Yanina, PL Gassman, and KM Rosso. 2008. "Bismuth Dimercaptopropanol (BisBAL) Inhibits the Expression of Extracellular Polysaccharides and Proteins by Brevundimonas diminuta: Implications for Membrane Microfiltration." *Biotechnology and Bioengineering* 99(3):634-643. doi:10.1002/bit.21615

Bae IT, Y Zhang, WJ Weber, M Ishimaru, Y Hirotsu, and M Higuchi. 2008. "Temperature Dependence of Electron-Beam Induced Effects in Amorphous Apatite." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 266(12-13):3037-3042. doi:10.1016/j.nimb.2008.03.160

Bae IT, Y Zhang, WJ Weber, M Ishimaru, Y Hirotsu, and M Higuchi. 2008. "Ionization-Induced Effects in Amorphous Apatite at Elevated Temperatures." *Journal of Materials Research* 23(4):962-967. doi:10.1557/JMR.2008.0114

Baer DR, JE Amonette, MH Engelhard, DJ Gaspar, AS Karakoti, SVNT Kuchibhatla, P Nachimuthu, J Nurmi, Y Qiang, V Sarathy, S Seal, A Sharma, PG Tratnyek, and CM Wang. 2008. "Characterization Challenges for Nanomaterials." *Surface and Interface Analysis* 40(3-4):529-537. doi:10.1002/sia.2726

Bagus PS, H Freund, H Kuhlenbeck, and ES Ilton. 2008. "A New Analysis of X-Ray Adsorption Branching Ratios: Use of Russell-Saunders Coupling." *Chemical Physics Letters* 455(4-6):331-334.

Bank TL, RK Kukkadapu, AS Madden, ME Baldwin, and PM Jardine. 2008. "Effects of Gamma-Sterilization on the Physico-Chemical Properties of Natural Sediments." *Chemical Geology* 251(1-4):1-7. doi:10.1016/j.chemgeo.2008.01.003

Beck KM, AG Joly, O Diwald, S Stankic, PE Trevisanutto, PV Sushko, AL Shluger, and WP Hess. 2008. "Energy and Site Selectivity in O-Atom Photodesorption from Nanostructured MgO." *Surface Science* 602(11):1968-1973. doi:10.1016/j.susc.2008.03.046

Bera D, S Kuchibhatla, S Azad, LV Saraf, CM Wang, V Shutthanandan, P Nachimuthu, DE Mccready, MH Engelhard, OA Marina, DR Baer, S Seal, and S Thevuthasan. 2008. "Growth and Characterization of Highly Oriented Gadolinia-Doped Ceria (111) Thin Films on Zirconia (111)/Sapphire (0001) Substrates." *Thin Solid Films* 516(18):6088-6094. doi:10.1016/j.tsf.2007.11.007

Boily JF, and AR Felmy. 2008. "On the Protonation of Oxo- and Hydroxo- Groups of the Goethite (a-FeOOH) Surface: A FTIR Spectroscopic Investigation of Surface O-H Stretching Vibrations." *Geochimica et Cosmochimica Acta* 72(14):3338-3357.

Boily JF, O Qafoku, and AR Felmy. 2007. "A Potentiometric, Spectrophotometric and Pitzer Ion-Interaction Study of Reaction Equilibria in the Aqueous H+-Al3+, H+-Oxalate and H+-Al3+-Oxalate Systems up to 5 mol*dm-3 NaCl ." *Journal of Solution Chemistry* 36(11-12):1727-1743. doi:10.1007/s10953-007-9203-9

Boily JF, J Szanyi, and AR Felmy. 2007. "Effects of Surface Coordination on the Temperature-Programmed Desorption of Oxalate from Goethite." *Journal of Physical Chemistry C* 111(45):17072-17081. doi:10.1021/jp075576q

Bondarchuk O, and I Lyubinetsky. 2007. "Preparation of $TiO_2$(110)-(1x1) Surface via UHV Cleavage: An Scanning Tunneling Microscopy Study." *Review of Scientific Instruments* 78(11): Art. No. 113907. doi:10.1063/1.2814160

Bonini N, M Lazzeri, N Marzari, and F Mauri. 2007. "Phonon Anharmonicities in Graphite and Graphene." *Physical Review Letters* 99(176802):1-4. doi:10.1103/PhysRevLett.99.176802

Bowers GM, DL Bish, and RJ Kirkpatrick. 2008. "$H_2O$ and Cation Structure and Dynamics in Expandable Clays: $^2H$ and $^{39}K$ NMR Investigations of Hectorite." *Journal of Physical Chemistry C* 112(16):6430-6438. doi:10.1021/jp7119087

Briknarova K, X Zhou, AC Satterthwait, DW Hoyt, KR Ely, and S Huang. 2008. "Structural Studies of the SET Domain from RIZ1 Tumor Suppressor." *Biochemical and Biophysical Research Communications* 366(3):807-813. doi:10.1016/j.bbrc.2007.12.034

Brusseau ML, EL Difilippo, C marble, and M Oostrom. 2008. "Mass-Removal and Mass-Flux-Reduction Behavior for Idealized Source Zones with Hydraulically Poorly-Accessible Immiscible Liquid." *Chemosphere* 71(8):1511-1521.

Bryantsev V, WA De Jong, KC Cossel, MS Diallo, WA Goddard III, GS Groenewold, W Chien, and MJ Van Stipdonk. 2008. "Two-Electron Three-Centered Bond in Side-On ($\eta$2) Uranyl(V) Superoxo Complexes." *Journal of Physical Chemistry A* 112(26):5777-5780. doi:10.1021/jp804202q

Buchko GW, and HJ Sofia. 2008. "Backbone $^1H$, $^{13}C$, and $^{15}N$ NMR assignments for the *Cyanothece* 51142 Protein cce_0567: A Protein Associated with Nitrogen Fixation in the DUF683 Family." *Biomolecular NMR Assignments* 2:25-28.

Buchko GW, H Robinson, HB Pakrasi, and MA Kennedy. 2008. "Insights into the Structural Variation between Pentapeptide Repeat Proteins - Crystal Structure of Rfr23 from *Cyanothece* 51142." *Journal of Structural Biology* 162(1):184-192.

Buchko GW, JG Bekhazi, JR Cort, NB Valentine, ML Snead, and WJ Shaw. 2008. "$^1H$, $^{13}C$, and $^{15}N$ Resonance Assignments of Murine Amelogenin, an Enamel Biomineralization Protein." *Biomolecular NMR Assignments* 2(1):89-91.

Buchko GW, O Litvinova, H Robinson, AF Yakunin, and MA Kennedy. 2008. "Functional and Structural Characterization of DR_0079 from *Deinococcus radiodurans*, a Novel Nudix Hydrolase with a Preference for Cytosine (Deoxy) Ribonucleoside 5'-di- and Triphosphates." *Biochemistry* 47(25):6571-82.

Bylaska EJ, M Dupuis, and PG Tratnyek. 2008. "One-Electron-Transfer Reactions of Polychlorinated Ethylenes: Concerted and Stepwise Cleavages." *Journal of Physical Chemistry A* 112(16):3712-3721.

Callister SJ, LA McCue, JE Turse, ME Monroe, KJ Auberry, RD Smith, JN Adkins, and MS Lipton. 2008. "Comparative Bacterial Proteomics: Analysis of the Core Genome Concept." *PLoS One* 3(2):e1542.

Bouchard LS, AO Sushkov, D Budker, J Ford, and AS Lipton. 2008. "Nuclear-Spin Relaxation of $^{207}Pb$ in Ferroelectric Powders." *Physical Review. A.* 77(2):Art. No. 022102. doi:10.1103/PhysRevA.77.022102

Chambers SA, SH Cheung, V Shutthanandan, S Thevuthasan, MK Bowman, and AG Joly. 2007. "Properties of Structurally Excellent N-doped $TiO_2$ Rutile." *Chemical Physics* 339(1-3):27-35. doi:10.1016/j.chemphys.2007.04.024

Chambers SA. 2007. "Surface Science Opportunities in the Electronic Structure of ZnO (A Perspective on the Article, "Quantitative Analysis of Surface Donors in ZnO", by D.C. Look)." *Surface Science* 601(23):5313-5314. doi:10.1016/j.susc.2007.10.004

Chang CL, MH Engelhard, and S Ramanathan. 2008. "Superior Nanoscale Passive Oxide Layers Synthesized Under Photon Irradiation for Environmental Protection." *Applied Physics Letters* 92(26):263103, 1-3.

Chang CL, MH Engelhard, and S Ramanathan. 2008. "Superior Nanoscale Passive Oxide Layers Synthesized Under Photon Irradiation for Environmental Protection." *Applied Physics Letters* 92(26):263103, 1-3.

Chen H, JA Lucas, WA Priyantha, M Kopczyk, RJ Smith, KR Lund, C Key, M Finsterbusch, PE Gannon, M Deibert, VI Gorokhovsky, V Shutthanandan, and P Nachimuthu. 2008. "Thermal Stability and Oxidation Resistance of TiCrAlYO Coatings on SS430 for Solid Oxide Fuel Cell Interconnect Applications." *Surface & Coatings Technology* 202(19):4820-4824.

Cheng C, JC Lehmann, and MH Engelhard. 2008. "Natural Oxidation of Black Carbon in Soils: Changes in Molecular Form and Surface Charge along a Climosequence." *Geochimica et Cosmochimica Acta* 72(6):1598-1610.

Cheng C, JC Lehmann, JE Thies, and SD Burton. 2008. "Stability of Black Carbon in Soils across a Climatic Gradient." *Journal of Geophysical Research. Biogeosciences* 113(G2):Art. No. G02027.

Cheng MD, E Corporan, MJ DeWitt, CW Spicer, MW Holdren, KA Cowen, A Laskin, DB Harris, RC Shores, RH Kagann, and RA Hashmonay. 2008. "Probing Emissions of Military Cargo Aircraft: Description of a Joint Field Measurement Strategic Environmental Research and Development Program." *EM: Air & Waste Management Association's Magazine for Environmental Managers* 58(6):787-796.

Cheng Y, J Hoard, C Lambert, JH Kwak, and CHF Peden. 2008. "NMR Studies of Cu/Zeolite SCR Catalysts Hydrothermally Aged with Urea." *Catalysis Today* 136(1-2):34-39. doi:10.1016/j.cattod.2008.01.019

Chen ZJ, HY Xiao, X Zu, L Wang, F Gao, J Lian, and RC Ewing. 2008. "Structural and Bonding Properties of Stannate Pyrochlores: A Density Functional Theory Investigation." *Computational Materials Science* 42(4):653-658. doi:10.1016/j.commatsci.2007.09.019

Cheung SH, P Nachimuthu, MH Engelhard, CM Wang, and SA Chambers. 2008. "N Incorporation, Composition and Electronic Structure in N-doped $TiO_2$(001) Anatase Epitaxial Films Grown on $LaAlO_3$(001)." *Surface Science* 602(1):133-141. doi:10.1016/j.susc.2007.09.061

Chimentão RJ, JE Herrera, JH Kwak, F Medina, Y Wang, and CHF Peden. 2007. "Oxidation of Ethanol to Acetaldehyde over Na-Promoted Vanadium Oxide Catalysts." *Applied Catalysis. A, General* 332(2):263-272. doi:10.1016/j.apcata.2007.08.024

Chorover J, S Choi, P Rotenberg, RJ Serne, N Rivera, CR Strepka, A Thompson, KT Mueller, and PA O'Day. 2008. "Silicon Control of Strontium and Cesium Partitioning in Hydroxide-Weathered Sediments." *Geochimica et Cosmochimica Acta* 72(8):2024-2047.

Cort JR, U Selan, A Schulte, F Grimm, MA Kennedy, and C Dahl. 2008. "Allochromatium Vinosum DsrC: Solution-State NMR Structure, Redox Properties and Interaction with DsrEFH, a Protein Essential for Purple Sulfur Bacterial Sulfur Oxidation." *Journal of Molecular Biology* 382:692-707. doi:10.1016/j.jmb.2008.07.022

Cygan RT, CT Stevens, RW Puls, SB Yabusaki, RD Wauchope, CJ McGrath, GP Curtis, MD Siegel, LA Veblen, and DR Turner. 2007. "Research Activities at U.S. Government Agencies in Subsurface Reactive Transport Modeling." *Vadose Zone Journal* 6(4):805-822. doi:10.2136/vzj2006.0091

Cui L, and LS Wang. 2008. "Stable Icosahedral Hollow Cage Clusters: Stannaspherene (Sn12 2-) and Plumbaspherene (Pb12 2-)." *International Reviews in Physical Chemistry* 27(1):139-166. doi:10.1080/01442350701791256

Cwiertny DM, J Baltrusaitis, GJ Hunter, A Laskin, M Scherer, and VH Grassian. 2008. "Characterization and Acid-Mobilization Study of Iron-Containing Mineral Dust Source Materials." *Journal of Geophysical Research. D. (Atmospheres)* 113(D5):Art. No. D05202. doi:10.1029/2007JD009332

Dagle RA, A Platon, A Datye, JM Vohs, Y Wang, and DR Palo. 2008. "PdZnAl Catalysts for the Reactions of Water-Gas-Shift, Methanol Steam Reforming, and Reverse-Water-Gas-Shift." *Applied Catalysis. A, General* 342(1-2):63-68. doi:10.1016/j.apcata.2008.03.005

Daly DS, KK Anderson, EA Panisko, SO Purvine, R Fang, ME Monroe, and SE Baker. 2008. "Mixed-Effects Statistical Model for Comparative LC-MS Proteomics Studies." *Journal of Proteome Research* 7(3):1209-1217. doi:10.1021/pr070441i

De Macedo LGM, and WA De Jong. 2008. "Fully Relativistic Calculations on the Potential Energy Surfaces of the Lowest 23 States of Molecular Chlorine." *Journal of Chemical Physics* 128(4):Art. No. 041101. doi:10.1063/1.2827457

De Silva MH, J Li, Z Zheng, and LR Corrales. 2008. "Correlation of Calculated Excited-state Energies and Experimental Quantum Yields of Luminescent Tb(III) β-diketonates." *Journal of Physical Chemistry A* 112(20):4527-4530. doi:10.1021/jp8002799

Devanathan R, A Venkatnathan, and M Dupuis. 2007. "Atomistic Simulation of Nafion Membrane. 2. Dynamics of Water Molecules and Hydronium Ions." *Journal of Physical Chemistry B* 111(45):13006-13013. doi:10.1021/jp0761057

Devanathan R, and WJ Weber. 2008. "Dynamic Annealing of Defects in Irradiated Zirconia-Based Ceramics." *Journal of Materials Research* 23(3):593-597. doi:10.1557/JMR.2008.0104

Ding J, CM Sorensen, N Jaitly, H Jiang, D Orton, ME Monroe, RJ Moore, RD Smith, and T Metz. 2008. "Application of the Accurate Mass and Time Tag Approach in Studies of the Human Blood Lipidome." *Journal of Chromatography B* 871(2):243-252. doi:10.1016/j.jchromb.2008.04.040

Dixon DA, T Wang, DJ Grant, KA Peterson, KO Christe, and GJ Schrobilgen. 2007. "Heats of Formation of Krypton Fluorides and Stability Predictions for $KrF_4$and $KrF_6$ from High Level Electronic Structure Calculations." *Inorganic Chemistry* 46(23):10016-10021. doi:10.1021/ic701313h

Doran JC, JD Fast, JC Barnard, A Laskin, Y Desyaterik, and MK Gilles. 2008. "Applications of Lagrangian Dispersion Modeling to the Analysis of Changes in the Specific Absorption of Elemental Carbon." *Atmospheric Chemistry and Physics* 8(5):1377-1389. www.atmos-chem.phys.net/8/1377/2008/

Du X, F Yang, NP Manes, DL Stenoien, ME Monroe, JN Adkins, DJ States, SO Purvine, DG Camp, II, and RD Smith. 2008. "Linear Discriminant Analysis - Based Estimation of the False Discovery Rate for Phosphopeptide Identifications." *Journal of Proteome Research* 7(6):2195-2203. doi:10.1021/pr070510t

Du X, SJ Callister, NP Manes, JN Adkins, RA Alexandridis, X Zeng, JH Roh, WE Smith, TJ Donohue, S Kaplan, RD Smith, and MS Lipton. 2008. "A Computational Strategy to Analyze Label-Free Temporal Bottom-up Proteomics Data." *Journal of Proteome Research* 7(7):2595-2604. doi:10.1021/pr0704837

Du Y, Z Dohnalek, and I Lyubinetsky. 2008. "Transient Mobility of Oxygen Adatoms upon $O_2$ Dissociation on Reduced $TiO_2$ (110)." *Journal of Physical Chemistry C* 112(7):2649-2653. doi:10.1021/jp077677u

Dumortier J, DN Streblow, AV Moses, JM Jacobs, CN Kreklywich, DG Camp, II, RD Smith, SL Orloff, and J Nelson. 2008. "Human Cytomegalovirus Secretome Contains Factors That Induce Angiogenesis and Wound Healing." *Journal of Virology* 82(13):6524-6535. doi:doi:10.1128/JVI.00502-08

Eggleston CM, J Voros, L Shi, BH Lower, TC Droubay, and PJ Colberg. 2008. "Binding and Direct Electrochemistry of OmcA, an Outer-Membrane Cytochrome from an Iron Reducing Bacterium, with Oxide Electrodes: A Candidate Biofuel Cell System." *Inorganica Chimica Acta* 361(3):769-777. doi:10.1016/j.ica.2007.07.015

Elias DA, SL Tollaksen, DW Kennedy, HM Mottaz, CS Giometti, JS McLean, EA Hill, GE Pinchuk, MS Lipton, JK Fredrickson, and YA Gorby. 2007. "The Influence of Cultivation Methods on Shewanella oneidensis Physiology and Proteome Expression." *Archives of Microbiology*. doi:10.1007/s00203-007-0321-y

Elias DA, SL Tollaksen, DW Kennedy, HM Mottaz, CS Giometti, JS Mclean, EA Hill, GE Pinchuk, MS Lipton, JK Fredrickson, and YA Gorby. 2008. "The Influence of Cultivation Methods on Shewanella oneidensis Physiology and Proteome Expression." *Archives of Microbiology* 189(4):313-324. doi:10.1007/s00203-007-0321-y

Engelmann MD, LA Metz, JE Delmore, MH Engelhard, and NE Ballou. 2008. "Electrodeposition of Technetium on Platinum for Thermal Ionization Mass Spectrometry (TIMS)." *Journal of Radioanalytical and Nuclear Chemistry* 276(2):493-498. doi:10.1007/s10967-008-0532-y

Epling WS, I Nova, and CHF Peden. 2008. "Preface." *Catalysis Today* 136(1-2):1-2. doi:10.1016/j.cattod.2008.03.008

Epling WS, CHF Peden, and J Szanyi. 2008. "Carbonate Formation and Stability on a Pt/BaO/$\gamma$-$Al_2O_3$ $NO_x$ Storage/Reduction Catalyst." *Journal of Physical Chemistry C* 112(29):10952-10959. doi:10.1021/jp712180q

Eraso JM, JH Roh, X Zeng, SJ Callister, MS Lipton, and S Kaplan. 2008. "Role of the Global Transcriptional Regulator PrrA in *Rhodobacter sphaeroides* 2.4.1: Combined Transcriptome and Proteome Analysis." *Journal of Bacteriology* 190(14):4831-4848. doi:10.1128/JB.00301-08

Fan PD, M Valiev, and K Kowalski. 2008. "Large-Scale Parallel Calculations with Combined Coupled Cluster and Molecular Mechanics Formalism: Excitation Energies of Zinc-Porphyrin in Aqueous Solution." *Chemical Physics Letters* 458(1-3):205-209.

Farber R. 2008. "GPGPUs: Neat Idea or Disruptive Technology." *Scientific Computing* 24(11).

Farber RM. 2008. "Storage in Transition." *Scientific Computing*.

Farber R. 2007. "The Future Looks Bright for Teraflop Computing." *Scientific Computing* 24(10):34.

Feng M, J Zhao, and H Petek. 2008. "Atomlike, Hollow-Core–Bound Molecular Orbitals of $C_{60}$." *Science* 320(5874):359-362. doi:10.1126/science.1155866

Fox III DN, I Le Trong, P Rajagopal, P Brzovic, RE Stenkamp, and RE Klevit. 2008. "Crystal Structure of the BARD1 Ankyrin Repeat Domain and Its Functional Consequences." *Journal of Biological Chemistry* 283(30):21179-21186. doi:10.1074/jbc.M802333200

Fredrickson JK, and JM Zachara. 2008. "Electron Transfer at the Microbe-Mineral Interface: A Grand Challenge in Biogeochemistry." *Geobiology* 6(3):245-253.

Gaan S, G Sun, K Hutches, and MH Engelhard. 2008. "Effect of Nitrogen Additives on Flame Retardant Action of Tributyl Phosphate: Phosphorus – Nitrogen Synergism." *Polymer Degradation and Stability* 93(1):99-108. doi:10.1016/j.polymdegradstab.2007.10.013

Gallagher NB, PL Gassman, and TA Blake. 2008. "Detection of Low Volatility Organic Analytes on Soils Using Infrared Reflection Spectroscopy." *Journal of Near Infrared Spectroscopy* 16(3):179-187. doi:10.1255/jnirs.776

Gallagher NB, PL Gassman, and TA Blake. 2008. "Strategies for Detecting Organic Liquids on Soils Using Mid-Infrared Reflection-Absorption Spectroscopy." *Environmental Science & Technology* 42(15):5700-5705. doi:10.1021/es8005404

Gan J, TR Allen, RC Birtcher, V Shutthanandan, and S Thevuthasan. 2008. "Radiation Effects on the Microstructure of a $^9$Cr-ODS Alloy." *JOM. The Journal of the Minerals, Metals and Materials Society* 60(1):24-28. doi:10.1007/s11837-008-0003-5

Gao F, Y Zhang, M Posselt, and WJ Weber. 2008. "Computational Study of Anisotropic Epitaxial Recrystallization in $^4$H-SiC." *Journal of Physics. Condensed matter* 20(12):Art. No. 125203. doi:10.1088/0953-8984/20/12/125203

Gardner JS, E Shurdha, CM Wang, LD Lau, RG Rodriguez, and JJ Pak. 2008. "Rapid Synthesis and Size Control of $CuInS_2$ Semi-Conductor Nanoparticles Using Microwave Irradiation." *Journal of Nanoparticle Research* 10(4):633-641. doi:10.1007/s11051-007-9294-7

Gibbs GV, RT Downs, DF Cox, NL Ross, MB Boisen, Jr., and KM Rosso. 2008. "Shared and Closed-Shell O-O Interactions in Silicates." *Journal of Physical Chemistry A* 112(16):3693-3699.

Gibbs GV, RT Downs, DF Cox, KM Rosso, NL Ross, A Kirfel, T Lippmann, W Morgenroth, and TD Crawford. 2008. "Experimental Bond Critical Point and Local Energy Density Properties Determined for Mn-O, Fe-O and Co-O Bonded Interactions for Tephroite, $Mn^2SiO_4$, fayalite, $Fe^2SiO_4$ and $Co^2SiO_4$ Olivine and Organic Metal Complexes: Comparison with Properties Calculated for Non-Transition and Transition Metal M-O Bonded Interactions for Silicates and Oxides." *Journal of Physical Chemistry A* 112(37):8811-8823. doi:10.1021/jp804280j

Glezakou VA, M Dupuis, and CJ Mundy. 2007. "Acid/Base Equilibria in Clusters and Their Role in Proton Exchange Membranes: Computational Insight." *Physical Chemistry Chemical Physics. PCCP* 9(43):5752-5760. doi:10.1039/b709752b

Goodman DW, CHF Peden, and MS Chen. 2007. "CO Oxidation on Ruthenium: The Nature of the Active Catalytic Surface." *Surface Science* 601(19):L124 - L126. doi:10.1016/j.susc.2007.08.003

Goodman DW, CHF Peden, and MS Chen. 2007. "Reply to Comment on "CO Oxidation on Ruthenium: The Nature of the Active Catalytic Surface" by H. Over, M. Muhler, and A.P. Seitsonen." *Surface Science* 601(23):5663–5665. doi:10.1016/j.susc.2007.09.042

Grate JW, OB Egorov, MJ O'Hara, and TA Devol. 2008. "Radionuclide Sensors for Environmental Monitoring: From Flow Injection Solid-Phase Absorptiometry to Equilibration-Based Preconcentrating Minicolumn Sensors with Radiometric Detection." *Chemical Reviews* 108(2):543-562. doi:10.1021/cr068115u

Grate JW. 2008. "Hydrogen-Bond Acidic Polymers for Chemical Vapor Sensing." *Chemical Reviews* 108(2):726-745. doi:10.1021/cr068109y

Grieves GA, NG Petrik, J Herring-Captain, B Olanrewaju, A Aleksandrov, RG Tonkyn, SE Barlow, GA Kimmel, and TM Orlando. 2008. "Photoionization of Sodium Salt Solutions in a Liquid Jet." *Journal of Physical Chemistry C* 112(22):8359-8364.

Groenewold GS, AK Gianotto, ME McIlwain, MJ Van Stipdonk, M Kullman, DT Moore, N Polfer, J Oomens, IA Infante, L Visscher, B Siboulet, and WA De Jong. 2008. "Infared Spectroscopy of Discrete Uranyl Anion Complexes." *Journal of Physical Chemistry A* 112(3):508-521. doi:10.1021/jp077309q

Groenewold GS, MJ Van Stipdonk, WA De Jong, J Oomens, GL Gresham, ME McIlwain, D Gao, B Siboulet, L Visscher, M Kullman, and N Polfer. 2008. "Infrared Spectroscopy of Dioxouranium (V) Complexes with Solvent Molecules: Effect of Reduction." *Chemphyschem* 9(9):1278-1285. doi:10.1002/cphc.200800034

Groenewold GS, J Oomens, WA De Jong, GL Gresham, ME McIlwain, and MJ Van Stipdonk. 2008. "Vibrational Spectroscopy of Anionic Nitrate Complexes of UO$_2$2+ and Eu$^3$+ Isolated in the Gas Phase." *Physical Chemistry Chemical Physics. PCCP* 10(8):1192-1202. doi:10.1039/b715337f

Hadjar O, JH Futrell, and J Laskin. 2007. "First Observation of Charge Reduction and Desorption Kinetics of Multiply Protonated Peptides Soft Landed onto Self-Assembled Monolayer Surfaces." *Journal of Physical Chemistry C* 111(49):18220-18225. doi:10.1021/jp075293y

Ham BM, F Yang, H Jayachandran, N Jaitly, ME Monroe, MA Gritsenko, EA Livesay, R Zhao, SO Purvine, D Orton, JN Adkins, DG Camp, II, SS Rossie, and RD Smith. 2008. "The Influence of Sample Preparation and Replicate Analyses on HeLa Cell Phosphoproteome Coverage." *Journal of Proteome Research* 7(6):2215-2221.

Hammond JR, WA De Jong, and K Kowalski. 2008. "Coupled-Cluster Dynamic Polarizabilities Including Triple Excitations." *Journal of Chemical Physics* 128:224102-1 - 224102-11. doi:10.1063/1.2929840

Hammond JR, K Kowalski, and WA de Jong. 2007. "Dynamic Polarizabilities of Polyaromatic Hydrocarbons Using Coupled-Cluster Linear Response Theory." *Journal of Chemical Physics* 127(14): Art. No. 144105. doi:10.1063/1.2772853

Han P, S Axnanda, I Lyubinetsky, and DW Goodman. 2007. "Atomic-Scale Assembly of a Heterogeneous Catalytic Site." *Journal of the American Chemical Society* 129(46):14355-14361. doi:10.1021/ja074891n

Hayes JA, DM Schubert, JE Amonette, P Nachimuthu, and RS Disselkamp. 2008. "Ultraviolet stimulation of hydrogen peroxide production using aminoindazole, diaminopyridine, and phenylenediamine solid polymer complexes of Zn(II)." *Journal of Photochemistry and Photobiology. A, Chemistry* 197(2-3):245-252. doi:10.1016/j.jphotochem.2007.12.031

Heikaus CC, JR Stout, MR Sekharan, CM Eakin, P Rajagopal, P Brzovic, JA Beavo, and RE Klevit. 2008. "Solution Structure of the cGMP Binding GAF Domain from

Phosphodiesterase 5: Insights into Nucleotide Specificity, Dimerization, and cGMP-Dependent Conformational Change." *Journal of Biological Chemistry* 283(33):22749-22759. doi:10.1074/jbc.M801577200

Henderson MA. 2008. "Effect of Coadsorbed Water on the Photodecomposition of Acetone on $TiO_2$(110)." *Journal of Catalysis* 256(2):287-292. doi:10.1016/j.jcat.2008.03.020

Hess NJ, ME Bowden, VM Parvanov, CJ Mundy, SM Kathmann, GK Schenter, and T Autrey. 2008. "Spectroscopic Studies of the Phase Transition in Ammonia Borane: Raman spectroscopy of single crystal NH3BH3 as a function of temperature from 88 to 330 K." *Journal of Chemical Physics* 128(3):Art. No. 034508. doi:10.1063/1.2820768

Hess NJ, MR Hartman, C Brown, E Mamontov, AJ Karkamkar, DJ Heldebrant, LL Daemen, and T Autrey. 2008. "Quasielastic neutron scattering of -NH3 and -BH3 rotational dynamics in orthorhombic ammonia borane." *Chemical Physics Letters* 459(1-6):85-88. doi:10.1016/j.cplett.2008.04.130

Hooker BS, DJ Bigelow, and CT Lin. 2007. "Methods for Mapping of Interaction Networks Involving Membrane Proteins." *Biochemical and Biophysical Research Communications* 363(3):457-461. doi:10.1016/j.bbrc.2007.09.031

Hopkins RJ, Y Desyaterik, AV Tivanski, RA Zaveri, CM Berkowitz, T Tyliszczak, MK Gilles, and A Laskin. 2008. "Chemical Speciation of Sulfur in Marine Cloud Droplets and Particles: Analysis of Individual Particles from the Marine Boundary Layer over the California Current." *Journal of Geophysical Research. D. (Atmospheres)* 113(D4):D04209. doi:10.1029/2007/JD008954

Hu JZ, DN Rommereim, KR Minard, A Woodstock, BJ Harrer, RA Wind, RP Phipps, and PJ Sime. 2008. "Metabolomics in Lung Inflammation: A High Resolution $^1$H NMR Study of Mice Exposed to Silica Dust ." *Toxicology Mechanisms and Methods* 18(5):385-398.

Hu JZ, JH Kwak, Z Yang, W Osborn, T Markmaitree, and LL Shaw. 2008. "Investigation of Mechanical Activation on Li-N-H Systems Using 6Li Magic Angle Spinning Nuclear Magnetic Resonance at Ultra-High Field." Journal of Power Sources 182(1):278-283.

Hu JZ, JH Kwak, Z Yang, W Osborn, T Markmaitree, and LL Shaw. 2008. "Probing the Reaction Pathway of Dehydrogenation of the LiNH2 + LiH Mixture Using In Situ 1H NMR Spectroscopy." Journal of Power Sources 181(1):116-119.

Huang H, M. Lin, XN Wang, T Kikuchi, HM Mottaz, AD Norbeck, and Y Rikihisa. 2008. "Proteomic Analysis of and Immune Responses to Ehrlichia chaffeensis Lipoproteins." Infection and Immunity 76:3405-3414. doi:10.1128/IAI.00056-08

Huang W, M Ji, CD Dong, X Gu, L Wang, XG Gong, and LS Wang. 2008. "Relativistic Effects and the Unique Low-Symmetry Structures of Gold Nanoclusters." *ACS Nano* 2(5):897-904. doi:10.1021/nn800074b

Ibrahim YM, ME Belov, AV Liyu, and RD Smith. 2008. "Automated Gain Control Ion Funnel Trap for Orthogonal Time-of-Flight Mass Spectrometry." *Analytical Chemistry* 80(14):5367-5376. doi:10.1021/ac8003488

Ibrahim Y, ME Belov, AV Tolmachev, DC Prior, and RD Smith. 2007. "Ion Funnel Trap Interface for Orthogonal Time-of-Flight Mass Spectrometry." *Analytical Chemistry* 79(20):7845-7852. doi:10.1021/ac071091m

Iddir H, V Komanicky, S Öğüt, H You, and P Zapol. 2007. "Shape of Platinum Nanoparticles Supported on $SrTiO_3$: Experiment and Theory." *Journal of Physical Chemistry C* 111(40):14782-14789. doi:10.1021/jp073041r

Ilton ES and PS Bagus. 2008. "Ligand Field Effects on the Multiplet Structure of the U4f XPS of $UO_2$." *Surface Science* 602(5):1114-1121. doi:10.1016/j.susc.2008.01.010

Ishimaru M, A Hirata, M Naito, IT Bae, Y Zhang, and WJ Weber. 2008. "Direct observations of thermally induced structural changes in amorphous silicon carbide." *Journal of Applied Physics* 104(3):033503, 1-5. doi:10.1063/1.2960342

Jackson VE, RN Craciun, DA Dixon, KA Peterson, and WA de Jong. 2008. "Prediction of Vibrational Frequencies of $UO_2^{2}+$ at the CCSD(T) Level." *Journal of Physical Chemistry A* 112(17):4095-4099. doi:10.1021/jp710334b

Jacob RE, G Laicher, and KR Minard. 2007. "3D MRI of Non-Gaussian $^3$He Gas Diffusion in the Rat Lung." *Journal of Magnetic Resonance* 188(2):357-366. doi:10.1016/j.jmr.2007.08.014

Jacobs JM, KM Waters, LE Kathmann, DG Camp, II, HS Wiley, RD Smith, and BD Thrall. 2008. "The Mammary Epithelial Cell Secretome and its Regulation by Signal Transduction Pathways." *Journal of Proteome Research* 7(2):558-569. doi:10.1021/pr0704377

Jensen J, Gö Possnert, and Y Zhang. 2008. "Temperature effect on low-k dielectric thin films studied by ERDA." *Journal of Physics: Conference Series* 100:012041. doi:10.1088/1742-6596/100/1/012041

Jin S, DS Daly, DL Springer, and JH Miller. 2008. "The effects of shared peptides on protein quantitation in label-free proteomics by LC/MS/MS." *Journal of Proteome Research* 7(1):164-169. doi:10.1021/pr0704175

Johnson KS, A Laskin, JL Jimenez, V Shutthanandan, LT Molina, D Salcedo, K Dzepina, and MJ Molina. 2008. "Comparative Analysis of Urban Atmospheric Aerosol by Proton-Induced X-ray Emission (PIXE), Proton Elastic Scattering Analysis (PESA), and Aerosol Mass Spectrometry (AMS)." *Environmental Science & Technology* 42(17):6619-6624. doi:10.1021/es800393e

Johnson RL, RB Thoms, RO Johnson, JT Nurmi, and PG Tratnyek. 2008. "Mineral Precipitation Upgradient from a Zero-Valent Iron Permeable Reactive Barrier." *Ground Water Monitoring and Remediation* 28(3):56-64.

Joly AG, KM Beck, and WP Hess. 2008. "Electronic Energy Transfer on CaO Surfaces." *Journal of Chemical Physics* 129(12):124704. doi:10.1063/1.2980049

Joly AG, W Chen, J Zhang, and SP Wang. 2007. "Electronic Energy Relaxation and Luminescence Decay Dynamics of $Eu^{3+}$ in $Zn_2SiO_4$:$Eu^{3+}$." *Journal of Luminescence* 126(2):491-496. doi:10.1016/j.jlumin.2006.09.004

Joslin EJ, LK Opresko, A Wells, HS Wiley, and DA Lauffenburger. 2007. "EGF-Receptor-Mediated Mammary Epithelial Cell Migration Is Driven by Sustained ERK Signaling from Autocrine Stimulation." *Journal of Cell Science* 120(20):3688-3699. doi:10.1242/jcs.010488

Kaiser NK, G Skulason, CR Weisbrod, S Wu, K Zhang, DC Prior, MA Buschbach, GA Anderson, and JE Bruce. 2008. "Restrained Ion Population Transfer: A Novel Ion Transfer Method for Mass Spectrometry." *Rapid Communications in Mass Spectrometry* 22(12):1955-1964.

Kamiya M, S Hirata, and M Valiev. 2008. "Fast Electron Correlation Methods for Molecular Clusters without Basis Set Superposition Errors." *Journal of Chemical Physics* 128(7):Art. No. 074103. doi:10.1063/1.2828517

Kannan S and M Zacharias. 2007. "Folding of a DNA Hairpin Loop Structure in Explicit Solvent Using Replica-Exchange Molecular Dynamics Simulations." *Biophysical Journal* 93:3218-3228. doi:10.1529/biophysj.107.108019

Karagulian F, AS Lea, CW Dilbeck, and BJ Finlayson-Pitts. 2008. "A New Mechanism for Ozonolysis of Unsaturated Organics on Solids: Phosphocholines on NaCl as A Model for Sea Salt particles." *Physical Chemistry Chemical Physics. PCCP* 10(4):528-541. doi:10.1039/b712715d

Karakoti AS, SVNT Kuchibhatla, KS Babu, and S Seal. 2007. "Direct Synthesis of Nanoceria in Aqueous Polyhydroxyl Solutions." *Journal of Physical Chemistry C* 111(46):17232-17240. doi:10.1021/jp076164k

Karakoti AS, S Kuchibhatla, DR Baer, S Thevuthasan, DC Sayle, and S Seal. 2008. "Self-Assembly of Cerium Oxide Nanostructures in Ice Molds." *Small* 4(8):1210-1216. doi:10.1002/smll.200800219

Kaspar TC, TC Droubay, SM Heald, MH Engelhard, P Nachimuthu, and SA Chambers. 2008. "Hidden Ferromagnetic Secondary Phases in Cobalt-doped ZnO Epitaxial Thin Films." Physical Review. B, Condensed Matter 77(20):201303. doi:10.1103/PhysRevB.77.201303

Kaspar TC, TC Droubay, Y Li, SM Heald, P Nachimuthu, CM Wang, V Shutthanandan, CA Johnson, DR Gamelin, and SA Chambers. 2008. "Lack of ferromagnetism in n-type cobalt-doped ZnO epitaxial thin films." *New Journal of Physics* 10(055010):1-16. doi:10.1088/1367-2630/10/5/055010

Kassianov EI, and M Ovtchinnikov. 2008. "On Reflectance Ratios and Aerosol Optical Depth Retrieval in the Presence of Cumulus Clouds ." *Geophysical Research Letters* 35(6):Art. No. L06807. doi:10.1029/2008GL033231

Kelly RT, JS Page, R Zhao, W Qian, HM Mottaz, K Tang, and RD Smith. 2008. "Capillary-Based Multi Nanoelectrospray Emitters: Improvements in Ion Transmission Efficiency and Implementation with Capillary Reversed-Phase LC-ESI-MS." *Analytical Chemistry* 80(1):143-149. doi:10.1021/ac701647s

Kerisit SN, NA Deskins, KM Rosso, and M Dupuis. 2008. "A Shell Model for Atomistic Simulation of Charge Transfer in Titania." *Journal of Physical Chemistry C* 112(20):7678-7688. doi:10.1021/jp8007865

Kim DH, YH Chin, JH Kwak, and CHF Peden. 2008. "Promotional Effects of H2O Treatment on NOx Storage over Fresh and Thermally Aged Pt-BaO/Al2O3 Lean NOx Trap Catalysts ." *Catalysis Letters* 124(1-2):39-45. doi:10.1007/s10562-008-9505-6

Kim DH, JH Kwak, J Szanyi, SJ Cho, and CHF Peden. 2008. "Roles of Pt and BaO in the Sulfation of Pt/BaO/$Al_2O_3$ Lean NOx Trap Materials: Sulfur K-edge XANES and Pt LIII XAFS Studies." *Journal of Physical Chemistry C* 112(8):2981-2987. doi:10.1021/jp077563i

Kim DH, JH Kwak, X Wang, J Szanyi, and CHF Peden. 2008. "Sequential high temperature reduction, low temperature hydrolysis for the regeneration of sulfated NOx trap catalysts." *Catalysis Today* 136(1-2):183-187. doi:10.1016/j.cattod.2007.12.134

Kim JY, M Engelhard, JP Choi, and KS Weil. 2008. "Effects of atmospheres on bonding characteristics of silver and alumina." *International Journal of Hydrogen Energy* 33(14):4001-4011. doi:10.1016/j.ijhydene.2007.12.042

Kim YK, BD Kay, JM White, and Z Dohnalek. 2008. "2-Propanol Dehydration on $TiO_2$(110): The Effect of Bridge-Bonded Oxygen Vacancy Blocking." *Surface Science* 602(2):511-516. doi:10.1016/j.susc.2007.10.049

Kim Y, BD Kay, JM White, and Z Dohnálek. 2007. "Alcohol Chemistry on Rutile $TiO_2$(110): The Influence of Alkyl Substituents on Reactivity and Selectivity." *Journal of Physical Chemistry C* 111(49):18236-18242. doi:10.1021/jp075608+

Kim Y, BD Kay, JM White, and Z Dohnálek. 2007. "Inductive Effect of Alkyl Chains on Alcohol Dehydration at Bridge-Bonded Oxygen Vacancies of $TiO_2$(110)." *Catalysis Letters* 119(1-2):1-4. doi:10.1007/s10562-007-9199-1

Kim YK, RJ Rousseau, BD Kay, JM White, and Z Dohnalek. 2008. "Catalytic Dehydration of 2-Propanol on (WO3)3 Clusters on TiO2(110)." *Journal of the American Chemical Society* 130(15):5059-5061. doi:10.1021/ja800730g

Kimmel GA, and NG Petrik. 2008. "Tetraoxygen on Reduced Ti02(110): Oxygen Adsorption and Reactions with Oxygen Vacancies." *Physical Review Letters* 100(19):Art. No. 196102. doi:10.1103/PhysRevLett.100.196102

Kirkpatrick RW, T Masiello, N Jariyasopit, A Weber, JW Nibler, A Maki, TA Blake, and TL Hubler. 2008. "High Resolution Infrared Spectroscopy of [1.1.1] Propellane." *Journal of Molecular Spectroscopy* 248(2):153-160.

Kleinman LI, SR Springston, PH Daum, YN Lee, LJ Nunnermacker, G Senum, JX Wang, J Weinstein-Lloyd, ML Alexander, JM Hubbe, JV Ortega, MR Canagaratna, and J Jayne. 2008. "The Time Evolution of Aerosol Composition Over the Mexico City Plateau." *Atmospheric Chemistry and Physics* 8(6):1559-1575.

Kokubo H, J Rösgen, DW Bolen, and BM Pettitt. 2007. "Molecular Basis of the Apparent Near Ideality of Urea Solutions." *Biophysical Journal* 93(10):3392-3407. doi:10.1529/biophysj.107.114181

Komlos J, Jr., AD Peacock, RK Kukkadapu, and PR Jaffe. 2008. "Long-Term Dynamics of Uranium Reduction/Reoxidation under Low Sulfate Conditions." *Geochimica et Cosmochimica Acta* 72(15):3603-3615. doi:10.1016/j.gca.2008.05.040

Kowalski K, JR Hammond, and WA de Jong. 2007. "Linear Response Coupled Cluster Singles and Doubles Approach with Modified Spectral Resolution of the Similarity Transformed Hamiltonian." *Journal of Chemical Physics* 127(16):164105 (9). doi:10.1063/1.2795708

Kowalski K, and M Valiev. 2008. "The Application of High-Level Iterative Coupled-Cluster Methods to the Cytosine Molecule." *Journal of Physical Chemistry A* 112(24):5538-5541.

Krzyminski KJ, M Jasionowski, and A Gutowska. 2008. "Reversible Sol-Gel Transitions in Aqueous Solutions of N-Isopropylacrylamide Ionic Copolymers ." *Polymer International* 57(4):592-604.

Kwak JH, JZ Hu, DH Kim, J Szanyi, and CHF Peden. 2007. "Penta-Coordinated $Al^{3+}$ Ions as Preferential Nucleation Sites for BaO on γ-$Al_2O_3$: An Ultra-High-Magnetic Field $^{27}Al$ MAS NMR Study." *Journal of Catalysis* 251(1):189-194. doi:10.1016/j.jcat.2007.06.029

Kwak JH, JZ Hu, AC Lukaski, DH Kim, J Szanyi, and CHF Peden. 2008. "The Role of PentaCoordinated Al3+ Ions in the High Temperature Phase Transformation of γ-Al2O3." *Journal of Physical Chemistry C* 112(25):9486–9492. doi:10.1021/jp802631u

Lane CD, NG Petrik, TM Orlando, and GA Kimmel. 2007. "Electron-Stimulated Oxidation of Thin Water Films Adsorbed on $TiO_2$(110)." *Journal of Physical Chemistry C* 111(44):16319-16329. doi:10.1021/jp072479o

Laskin J, P Wang, and O Hadjar. 2008. "Soft-Landing of Peptide Ions Onto Self-Assembled Monolayer Surfaces: an Overview." *Physical Chemistry Chemical Physics. PCCP* 10(8):1079-1090. doi:10.1039/b712710c

Laskin J, Z Yang, and IK Chu. 2008. "Energetics and Dynamics of Electron Transfer and Proton Transfer in Dissociation of Metal III (salen)-Peptide Complexes in the Gas Phase." *Journal of the American Chemical Society* 130(10):3218-3230. doi:10.1021/ja077690s

Lau K, W Zheng, N Wong, and W Li. 2007. "Theoretical Prediction of the Ionization Energies of the $C_4H_7$ Radicals: 1-Methylallyl, 2-Methylallyl, Cyclopropylmethyl, and Cyclobutyl Radicals." *Journal of Chemical Physics* 127:154302. doi:10.1063/1.2774972

Lebarbier V, R Dagle, T Conant, JM Vohs, AK Datye, and Y Wang. 2008. "CO/FTIR Spectroscopic Characterization of Pd/ZnO/$Al_2O_3$ Catalysts for Methanol Steam Reforming." *Catalysis Letters* 112:223-227. doi:10.1007/s10562-008-9407-7

Lee AC, G Liu, CK Heng, SN Tan, TM Lim, and Y Lin. 2008. "Sensitive electrochemical detection of horseradish peroxidase at disposable screen-printed carbon electrode." *Electroanalysis* 20(18):2040-2046. doi:DOI: 10.1002/elan.200804287

Lee J, Y Lee, JK Youn, HB Na, T Yu, H Kim, S Lee, Y Koo, JH Kwak, HG Park, HN Chang, M Hwang, JG Park, J Kim, and T Hyeon. 2008. "Simple Synthesis of Functionalized Superparamagnetic Magnetite/Silica Core/Shell Nanoparticles and their Application as Magnetically Separable High-Performance Biocatalysts." *Small* 4(1):143-152. doi:10.1002/smll.200700456

Li G, D Hu, GG Xia, JM White, and ZC Zhang. 2008. "High Throughput Operando Studies using Fourier Transform Infrared Imaging and Raman Spectroscopy." *Review of Scientific Instruments* 79:074101. doi:10.1063/1.2949389

Li S, and DA Dixon. 2007. "Low-Lying Electronic States of $M_3O_9^-$ and $M_3O_9^{2-}$ (M = Mo, W)." *Journal of Physical Chemistry A* 111(43):11093-11099. doi:10.1021/jp074187t

Li SC, Z Zhang, D Sheppard, BD Kay, JM White, Y Du, I Lyubinetsky, GA Henkelman, and Z Dohnalek. 2008. "Intrinsic Diffusion of Hydrogen on Rutile TiO2(110)." *Journal of the American Chemical Society* 130(28):9080-9088. doi:10.1021/ja8012825

Li XS, GE Fryxell, CM Wang, and MH Engelhard. 2008. "The Synthesis of Ag-Doped Mesoporous TiO2 ." *Microporous and Mesoporous Materials* 111(1-3):639-642. doi:10.1016/j.micromeso.2007.07.042

Li Y, TC Kaspar, TC Droubay, Z Zhu, V Shutthanandan, P Nachimuthu, and SA Chambers. 2008. "Electronic properties of H and D doped ZnO epitaxial films." *Applied Physics Letters* 92(15):Art. No. 152105.

Lin YY, G Liu, CM Wai, and Y Lin. 2008. "Bioelectrochemical Immunoassay of Polychlorinated Biphenyl." *Analytica Chimica Acta* 612:23-28. doi:10.1016/j.aca.2008.01.080

Lin YY, J Wang, G Liu, H Wu, CM Wai, and Y Lin. 2008. "A nanoparticle label/immunochromatographic electrochemical biosensor for rapid and sensitive detection of prostate-specific antigen ." *Biosensors and Bioelectronics* 23(11):1659-1665.

Lins RD, ER Vorpagel, M Guglielmi, and TP Straatsma. 2008. "Computer Simulation of Uranyl Uptake by the Rough Lipopolysaccharide Membrane of Pseudomonas aeruginosa." *Biomacromolecules* 9(1):29-35. doi:10.1021/bm700609r

Lipton AS, MM Morlok, G Parkin, and PD Ellis. 2008. "67Zn Solid-State NMR Spectroscopy of {[TpBut,Me]Zn(OH2)}[HOB(C6F5)3]. The Importance of the Anion [HOB(C6F5)3]-." *Inorganic Chemistry* 47(12):5184-5189. doi:10.1021/ic800009b

Lipton AS, RW Heck, M Hernick, CA Fierke, and PD Ellis. 2008. "Residue Ionization in LpxC Directly Observed by 67Zn NMR Spectroscopy." *Journal of the American Chemical Society* 130(38):12671-12679. doi:10.1021/ja801776c

Lipton AS, RW Heck, SV Primak, DR McNeill, DM Wilson Iii, and PD Ellis. 2008. "Characterization of $Mg^{2+}$ Binding to the DNA Repair Protein Apurinic/Apyrimidic Endonuclease 1 via Solid-State $^{25}Mg$ NMR Spectroscopy." *Journal of the American Chemical Society* 130(29):9332-9341. doi:10.1021/ja0776881

Lipton AS, RW Heck, GR Staeheli, M Valiev, WA De Jong, and PD Ellis. 2008. "A QM/MM Approach to Interpreting Zn-67 Solid-State NMR data in Zinc Proteins." *Journal of the American Chemical Society* 130(19):6224-6230.

Liu C, JM Zachara, NS Foster, and J Strickland. 2007. "Kinetics of Reductive Dissolution of Hematite by Bioreduced Anthraquinone-2,6-Disulfonate." *Environmental Science & Technology* 41(22):7730-7735. doi:10.1021/es070768k

Liu C, JM Zachara, N Qafoku, and Z Wang. 2008. "Scale-Dependent Desorption of Uranium from Contaminated Subsurface Sediments." *Water Resources Research* 44:W08413. doi:10.1029/2007WR006478

Liu G, and Y Lin. 2007. "Nanomaterial Labels in Electrochemical Immunosensors and Immunoassays." *Talanta* 74(3):308-317. doi:10.1016/j.talanta.2007.10.014

Liu G, Y Lin, H Wu, and Y Lin. 2007. "Voltammetric Detection of Cr (VI) with Disposable Screen-Printed Electrode Modified with Gold Nanoparticles." *Environmental Science & Technology* 41(23):8129-8134. doi:10.1021/es071726z

Liu G, Y Lin, J Wang, H Wu, CM Wai, and Y Lin. 2007. "Disposable Electrochemical Immunosensor Diagnosis Device Based on Nanoparticle Probe and Immunochromatographic Strip." *Analytical Chemistry* 79(20):7644-7653. doi:10.1021/ac070691i

Liu S, and N Govind. 2008. "Toward Understanding the Nature of Internal Rotation Barriers with a New Energy Partition Scheme: Ethane and n-Butane." *Journal of Physical Chemistry A* 112(29):6690-6699. doi:10.1021/jp800376a

Liu S, N Govind, and L Pedersen. 2008. "Exploring the Origin of the Internal Rotational Barrier for Molecules with One Rotatable Dihedral Angle." *Journal of Chemical Physics* 129(9):094104-1 - 094104-10. doi:10.1063/1.2976767

Liu Y, JP Cain, H Wang, and A Laskin. 2007. "Kinetic Study of Heterogeneous Reaction of Deliquesced NaCI Particles with Gaseous HNO3 Using Particle-on-Substrate Stagnation Flow Reactor Approach." *Journal of Physical Chemistry A* 111(40):10026-10043. doi:10.1021/jp072005p

Liu Y, W Chen, S Wang, AG Joly, SL Westcott, and BK Woo. 2008. "X-Ray Luminescence of LaF3:Tb3+ and LaF3:Ce3+, Tb3+ Water Soluble Nanoparticles." *Journal of Applied Physics* 103(6):Art. No. 063105. doi:10.1063/1.2890148

Liu Y, W Chen, S Wang, and AG Joly. 2008. "Investigation of Water-Soluble X-ray Luminescence Nanoparticles for Photodynamic Activation." *Applied Physics Letters* 92(4):Art. No. 043901.

Liu Y, ER Gibson, JP Cain, H Wang, VH Grassian, and A Laskin. 2008. "Kinetics of Heterogeneous Reaction of $CaCO_3$ Particles with Gaseous $HNO_3$ Over a Wide Range of Humidity." *Journal of Physical Chemistry A* 112(7):1561-1571. doi:10.1021/jp076169H

Liu Y, RE Miller, T Zhang, Q Feng, W Votava, D Li, LN Dunkleberger, X Wang, R Gray, T Bibens, J Helfer, K Mooney, R Nowak, P Lubitz, and Y Zhang. 2008. "Coatings of Fe/FeAIN Thin Films." *Journal of the American Ceramic Society* 27(3):265-275.

Liu Y, Z Yang, Y Desyaterik, PL Gassman, H Wang, and A Laskin. 2008. "Hygroscopic Behavior of Substrate-Deposited Particles Studied by Micro-FT-IR Spectroscopy and Complementary Methods of Particle Analysis." *Analytical Chemistry* 80(3):633-642. doi:10.1021/ac701638r

Livesay EA, K Tang, BK Taylor, MA Buschbach, DF Hopkins, BL LaMarche, R Zhao, Y Shen, DJ Orton, RJ Moore, RT Kelly, HR Udseth, and RD Smith. 2008. "Fully Automated Four-Column Capillary LC-MS System for Maximizing Throughput in Proteomic Analyses." *Analytical Chemistry* 80(1):294-302. doi:10.1021/ac701727r

Lopez-Ferrer D, K Petritis, KK Hixson, TH Heibeck, RJ Moore, ME Belov, DG Camp, II, and RD Smith. 2008. "Application of pressurized solvents for ultra fast trypsin hydrolysis in proteomics: Proteomics on the fly." *Journal of Proteome Research* 7(8):3276-3281. doi:10.1021/pr7008077

Lopez-Ferrer D, TH Heibeck, K Petritis, KK Hixson, W Qian, ME Monroe, AM Mayampurath, RJ Moore, ME Belov, DG Camp, II, and RD Smith. 2008. "Rapid Sample Processing For LC-MS Based Quantitative Proteomics Using High Intensity

Focused Ultrasounds." *Journal of Proteome Research* 7(9):3860-3867. doi:10.1021/pr800161x

Lower BH, RD Lins, ZW Oestreicher, TP Straatsma, MF Hochella Jr., L Shi, and SK Lower. 2008. "In Vitro Evolution of a Peptide with a Hematite Binding Motif That May Constitute a Natural Metal-Oxide Binding Archetype." *Environmental Science & Technology* 42(10):3821-3827. doi:10.1021/es702688c

Ma L, Y Wang, J Xue, Q Chen, W Zhang, and W Zhang. 2007. "Energy Loss and Straggling of MeV Ions through Biological Samples." *Journal of Applied Physics* 102(8):084702, 1-6. doi:10.1063/1.2800996

Majors PD, JS Mclean, and JC Scholten. 2008. "NMR bioreactor development for live in-situ microbial functional analysis." *Journal of Magnetic Resonance* 192(1):159-166. doi:10.1016/j.jmr.2008.02.014

Manes NP, RD Estep, HM Mottaz, RJ Moore, TRW Clauss, ME Monroe, X Du, JN Adkins, S Wong, and RD Smith. 2008. "Comparative Proteomics of Human Monkeypox and Vaccinia Intracellular Mature and Extracellular Enveloped Virions." *Journal of Proteome Research* 3:960-8. doi:10.1021/pr070432+

Marginean N, RT Kelly, JS Page, K Tang, and RD Smith. 2007. "Electrospray Characteristic Curves: In Pursuit of Improved Performance in the Nanoflow Regime." *Analytical Chemistry* 79(21):8030-8036. doi:10.1021/ac0707986

Marginean I, RT Kelly, DC Prior, BL Lamarche, K Tang, and RD Smith. 2008. "Analytical Characterization of the Electrospray Ion Source in the Nanoflow Regime." *Analytical Chemistry* 80(17):6573-6579. doi:10.1021/ac800683s

Markowitz VM, E Szeto, K Palaniappan, Y Grechkin, K Chu, IMA Chen, I Dubchak, I Anderson, A Lykidis, K Mavromatis, NN Ivanova, and NC Kyrpides. 2008. "The Integrated Microbial Genomes (IMG) System in 2007: Data Content and Analysis Tool Extensions." *Nucleic Acids Research* 36(1):D528-D533. doi:10.1093/nar/gkm846

Markowitz VM, NN Ivanova, E Szeto, K Palaniappan, K Chu, D Dalevi, IMA Chen, Y Grechkin, I Dubchak, I Anderson, A Lykidis, K Mavromatis, P Hugenholtz, and NC Kyrpides. 2008. "IMG/M: A Data Management and Analysis System for Metagenomes." *Nucleic Acids Research* 36(1):D534-D538. doi:10.1093/nar/gkm869

Marshall MJ, AE Plymale, DW Kennedy, L Shi, Z Wang, SB Reed, AC Dohnalkova, CJ Simonson, C Liu, DA Saffarini, MF Romine, JM Zachara, AS Beliaev, and JK Fredrickson. 2008. "Hydrogenase- and Outer Membrane c-Type Cytochrome-Facilitated Reduction of Technetium(VII) by Shewanella oneidensis MR-1." *Environmental Microbiology* 10(1):125-136. doi:10.1111/j.1462-2920.2007.01438.x

Marsili E, H Beyenal, L Di Palma, C Merli, A Dohnalkova, JE Amonette, and Z Lewandowski. 2007. "Uranium Immobilization by Sulfate-Reducing Biofilms Grown on Hematite, Dolomite, and Calcite." *Environmental Science & Technology* 41(24):8349-8354. doi:10.1021/es071335k

Martinez SE, CC Heikaus, RE Klevit, and JA Beavo. 2008. "The Structure of the GAF A Domain from Phosphodiesterase 6c Reveals Determinants of cGMP Binding, a Conserved Binding Surface, and a Large cGMP-Dependent Conformational Change." *Journal of Biological Chemistry* 283(38):25913-25919. doi:10.1074/jbc.M802891200

Mayampurath AM, N Jaitly, SO Purvine, ME Monroe, KJ Auberry, JN Adkins, and RD Smith. 2008. "DeconMSn: A Software Tool for accurate parent ion monoisotopic mass determination for tandem mass spectra." *Bioinformatics* 24(7):1021-1023. doi:10.1093/bioinformatics/btn063

McKinley JP, JM Zachara, J Wan, DE McCready, and SM Heald. 2007. "Geochemical Controls on Contaminant Uranium in Vadose Hanford Formation Sediments at the 200 Area and 300 Area, Hanford Site, Washington." *Vadose Zone Journal* 6(4):1004-1017. doi:10.2136/vzj2006.0184

McLean JS, PD Majors, CL Reardon, CL Bilskis, SB Reed, MF Romine, and JK Fredrickson. 2008. "Investigations of Structure and Metabolism within Shewanella oneidensis MR-1 Biofilms ." *Journal of Microbiological Methods* 74(1):47-56.

McLean JS, O Ona, and PD Majors. 2008. "Correlated Biofilm Imaging, Transport and Metabolism Measurements via Combined Nuclear Magnetic Resonance and Confocal Microscopy." *The ISME Journal* 2(2):121-131. doi:10.1038/ismej.2007.107

McLean JS, GE Pinchuk, OV Geydebrekht, CL Bilskis, BA Zakrajsek, EA Hill, D Saffarini, MF Romine, YA Gorby, JK Fredrickson, and AS Beliaev. 2008. "Oxygen-dependent autoaggregation in Shewanella oneidensis MR-1." *Environmental Microbiology* 10(7):1861-1876. doi:10.1111/j.1462-2920.2008.01608.x

Mei D, NA Deskins, and M Dupuis. 2007. "A Density Functional Theory Study of Formaldehyde Adsorption on Ceria." *Surface Science* 601(21):4993-5001. doi:10.1016/j.susc.2007.08.027

Mei D, NA Deskins, M Dupuis, and Q Ge. 2008. "Density Functional Theory Study of Methanol Decomposition on the $CeO_2$(110) Surface ." *Journal of Physical Chemistry C* 112(11):4257-4266.

Metz T, JS Page, ES Baker, K Tang, J Ding, Y Shen, and RD Smith. 2008. "High Resolution Separations and Improved Ion Production and Transmission in Metabolomics." *Trends in Analytical Chemistry. TrAC* 27(3):205-214. doi:10.1016/j.trac.2007.11.003

Metz T, W Qian, JM Jacobs, MA Gritsenko, RJ Moore, AD Polpitiya, ME Monroe, DG Camp, II, PW mueller, and RD Smith. 2008. "Application of Proteomics in the Discovery of Candidate Protein Biomarkers in a Diabetes Autoantibody Standardization Program Sample Subset." *Journal of Proteome Research* 7(2):698-707. doi:10.1021/pr700606w

Miller JH, S Jin, WF Morgan, A Yang, Y Wan, JS Peters, and DL Springer. 2008. "Profiling mitochondrial proteins in radiation-induced genome-unstable cell lines with persistent oxidative stress by mass spectrometry." *Radiation Research* 169(6):700-706.

Misra SK, SI Andronenko, MH Engelhard, AP Thurber, KM Reddy, and A Punnoose. 2008. "Role of dopant incorporation on the magnetic properties of Ce1-xNixO2 nanoparticles: An electron paramagnetic resonance study." *Journal of Applied Physics* 103(7):Art. No. 07D122.

Nichols P, EJ Bylaska, GK Schenter, and WA De Jong. 2008. "Equatorial and Apical Solvent Shells of the $UO_2^{2+}$ Ion." *Journal of Chemical Physics* 128(12):124507. doi:10.1063/1.2884861

Mohanty SR, B Kollah, DB Hedrick, AD Peacock, RK Kukkadapu, and EE Roden. 2008. "Biogeochemical Processes In Ethanol Stimulated Uranium Contaminated Subsurface Sediments." *Environmental Science & Technology* 42(12):4384-4390.

Ney A, K Ollefs, S Ye, T Kammermeier, V Ney, TC Kaspar, SA Chambers, F Wilhelm, and A Rogalev. 2008. "Absence of Intrinsic Ferromagnetic Interactions of Isolated and Paired Co Dopant Atoms in Zn1−xCoxO with High Structural Perfection." *Physical Review Letters* 100(15):Art. No. 157201. doi:10.1103/PhysRevLett.100.157201

Nguyen BT, JC Lehmann, J Kinyangi, R Smernik, and MH Engelhard. 2008. "Long-term Black Carbon Dynamics in Cultivated Soil." *Biogeochemistry* 89(3):295-308. doi:10.1007/s10533-008-9220-9

Ohno T, Z Wang, and R Bro. 2008. "PowerSlicing to determine fluorescence lifetimes of water-soluble organic matter derived from soils, plant biomass, and animal manures." *Analytical and Bioanalytical Chemistry* 390(8):2189-2194. doi:10.1007/s00216-008-1963-6

Oostrom M, ML Rockhold, PD Thorne, MJ Truex, GV Last, and VJ Rohay. 2007. "Carbon Tetrachloride Flow and Transport in the Subsurface of the 216-Z-9 Trench at the Hanford Site." *Vadose Zone Journal* 6(4):971-984. doi:10.2136/vzj2006.0166

Ouyang J, JA Ripmeester, X Wu, D Kingston, K Yu, AG Joly, and W Chen. 2007. "Upconversion Luminescence of Colloidal CdS and ZnCdS Semiconductor Quantum Dots." *Journal of Physical Chemistry C* 111(44):16261-16266. doi:10.1021/jp074416b

Ozensoy E, DR Herling, and J Szanyi. 2008. "NOx Reduction on a Transition Metal-free γ-Al2O3 Catalyst Using Dimethylether (DME)." *Catalysis Today* 136(1-2):46-54.

Pal R, L Cui, S Bulusu, HJ Zhai, LS Wang, and XC Zeng. 2008. "Probing the Electronic and Structural Properties of Doped Aluminium Clusters: MAI12-(M=Li,Cu, and Au)." *Journal of Chemical Physics* 128(2):Art. No. 024305. doi:10.1063/1.2805386

Pan LL, J Li, and LS Wang. 2008. "Low-Lying Isomers of the B9- Boron Cluster: The Planar Molecular Wheel Versus Three-Dimensional Structures." *Journal of Chemical Physics* 129(2):024302. doi:10.1063/1.2948405

Paxton WF, MJ O'Hara, SM Peper, SL Petersen, and JW Grate. 2008. "Accelerated Analyte Uptake on Single Beads in Microliter-scale Batch Separations using Acoustic Streaming: Plutonium Uptake by Anion Exchange for Analysis by Mass Spectrometry." *Analytical Chemistry* 80(11):4070-4077. doi:10.1021/ac800160n

Pelletier DA, GB Hurst, LJ Foote, PK Lankford, CK McKeown, TYS Lu, DD Schmoyer, MB Shah, WJ Hervey IV, WH McDonald, BS Hooker, WR Cannon, DS Daly, JM Gilmore, HS Wiley, DL Auberry, Y Wang, F Larimer, SJ Kennel, MJ Doktycz, J Morrell-Falvey, ET Owens, and MV Buchanan. 2008. "A general system for studying protein-protein interactions in gram-negative bacteria." *Journal of Proteome Research* 7(8):3319-3328. doi:10.1021/pr8001832

Peretyazhko T, JM Zachara, SM Heald, BH Jeon, RK Kukkadapu, C Liu, DA Moore, and CT Resch. 2008. "Heterogeneous Reduction of Tc(VII) by Fe(II) at the Solid-Water Interface." *Geochimica et Cosmochimica Acta* 72(6):1521-1539. doi:10.1016/j.gca.2008.01.004

Peretyazhko T, JM Zachara, SM Heald, RK Kukkadapu, C Liu, AE Plymale, and CT Resch. 2008. "Reduction of Tc(VII) by Fe(II) Sorbed on Al (hydr)oxides." *Environmental Science & Technology* 42(15):5499-5506. doi:10.1021/es8003156

Pertz OC, Y Wang, F Yang, W Wang, LJ Gay, MA Gritsenko, TR Clauss, DJ Anderson, T Liu, KJ Auberry, DG Camp, II, RD Smith, and RL Klemke. 2008. "Spatial Mapping of the Neurite and Soma Proteomes Reveals a Functional Cdc42/Rac Regulatory Network." *Proceedings of the National Academy of Sciences of the United States of America* 105(6):1931-1936. doi:10.1073/pnas.0706545105

Petrik NG, and GA Kimmel. 2007. "Hydrogen Bonding, H-D Exchange, and Molecular Mobility in Thin Water Films on $TiO_2$(110)." *Physical Review Letters* 99(19):Art.No.196103. doi:10.1103/PhysRevLett.99.196103

Petyuk VA, N Jaitly, RJ Moore, J Ding, TO Metz, K Tang, ME Monroe, AV Tolmachev, JN Adkins, ME Belov, AR Dabney, W Qian, DG Camp, II, and RD Smith. 2008. "Elimination of Systematic Mass Measurement Errors in Liquid Chromatography-Mass Spectrometry Based Proteomics using Regression Models and *a Priori* Partial Knowledge of the Sample Content." *Analytical Chemistry* 80(3):693-706. doi:10.1021/ac701863d

Pierce EM, EA Cordova, LJ Calligan, WJ Shaw, and BP McGrail. 2008. "An Experimental Study of the Dissolution Rates of Simulated Aluminoborosilicate Waste Glasses as a Function of pH and Temperature under Dilute Conditions." *Applied Geochemistry* 23(9):2559-2573. doi:doi:10.1016/j.apgeochem.2008.05.006

Pierce EM, EL Richards, AM Davis, LR Reed, and EA Cordova. 2008. "Aluminoborosilicate Waste Glass Dissolution under Alkaline Conditions at 40°C:

Implications for a Chemical Affinity-Based Rate Equation." *Environmental Chemistry* 5(1):73-85. doi:10.1071/EN07058

Polpitiya AD, W Qian, N Jaitly, VA Petyuk, JN Adkins, DG Camp, II, GA Anderson, and RD Smith. 2008. " DAnTE: a statistical tool for quantitative analysis of –omics data." *Bioinformatics* 24(13):1556-1558. doi:10.1093/bioinformatics/btn217

Posselt M, F Gao, and H Bracht. 2008. "Correlation between Self-Diffusion and the Migration Mechanisms of Point Defects in Si: An Atomistic Study." *Physical Review. B, Condensed Matter* 78:035208. doi:10.1103/PhysRevB.78.035208

Priyantha WA, H Chen, M Kopczyk, RJ Smith, AN Kayani, A Comouth, M Finsterbusch, P Nachimuthu, and DE Mccready. 2008. "Interface Mixing of Al/Fe and Fe/Al Bilayer Systems and the Role of Ti as a Stabilizing Interlayer using Rutherford Backscattering Spectrometry and X-Ray Reflectometry." *Journal of Applied Physics* 103(1):Art. No. 014508. doi:10.1063/1.2829803

Puzon GJ, YC Huang, A Dohnalkova, and L Xun. 2008. "Isolation and characterization of an NAD+-degrading bacterium PTX1 and its role in chromium biogeochemical cycle." *Biodegradation* 19(3):417-424. doi:10.1007/s10532-007-9147-1

Rai D, DA Moore, KM Rosso, AR Felmy, and H Bolton, Jr. 2008. "Environmental Mobility of Pu(IV) in the Presence of Ethylenediaminetetraacetic Acid: Myth or Reality." *Journal of Solution Chemistry* 37(7):957-986. doi:10.1007/s10953-008-9282-2

Ramana CV, U Becker, V Shutthanandan, and CM Julien. 2008. "Oxidation and Metal-Insertion in Molybdenite Surfaces: Evaluation of Charge-Transfer Mechanisms and Dynamics ." *Geochemical Transactions* 9(8):1-8. doi:doi:10.1186/1467-4866-9-8

Redington RL, TE Redington, and RL Sams. 2008. "Tunneling Splittings for "O...O Stretching" and Other Vibrations of Tropolone Isotopomers Observed in the Infrared Spectrum Below 800 cm-1." *Journal of Physical Chemistry A* 112(7):1480-1492. doi:10.1021/jp0757255

Riley BJ, SK Sundaram, BR Johnson, and LV Saraf. 2007. "Differential Etching of Chalcogenides for Infrared Photonic Waveguide Structures." *Journal of Non-Crystalline Solids* 354(10-11):813-816. doi:10.1016/j.jnoncrysol.2007.08.061

Rong Z, F Gao, WJ Weber, and G Hobler. 2007. "Monte Carlo Simulations of Defect Recovery within a 10 keV Collision Cascade in 3C-SiC." *Journal of Applied Physics* 102(10):103508, 1-7. doi:10.1063/1.2812701

Saheb AH, JA Smith, M Josowicz, J Janata, DR Baer, and MH Engelhard. 2008. "Controlling Size of Gold Clusters in Polyaniline from Top-Down and from Bottom-Up." *Journal of Electroanalytical Chemistry* 621(2):238-244. doi:10.1016/j.jelechem.2007.11.025

Sani R, BM Peyton, and A Dohnalkova. 2008. "Comparison of uranium(VI) removal by Shewanella oneidensis MR-1 in flow and batch reactors." *Water Research* 42(12):2993-3002. doi:10.1016/j.watres.2008.04.003

Saraf LV, CM Wang, MH Engelhard, and P Nachimuthu. 2008. "Surface & Interface Properties of 10-12 Unit Cells Thick Sputter Deposited Epitaxial CeO2 Films." *Research Letters in Materials Science* 2008:5 pages doi:10115/2008/206019. doi:Article ID 206019

Sarathy V, PG Tratnyek, J Nurmi, DR Baer, JE Amonette, CL Chun, RL Penn, and EJ Reardon. 2008. "Aging of Iron Nanoparticles in Aqueous Solution: Effects on Structure and Reactivity." *Journal of Physical Chemistry C* 112(7):2286-2293. doi:10.1021/jp0777418

Sayle DC, BC Mangili, DW Price, AS Karakoti, S Kuchibhatla, S Seal, Q Hao, Z Wang, X Xu, G Mobus, and TX Sayle. 2008. "Mapping Nanostructure: A Systematic Enumeration of Nanomaterials by Assembling Nanobuilding Blocks at Cystallographic Positions." *ACS Nano* 2(6):1237-1251. doi:10.1021/nn800065g

Scheibe TD, P Meakin, PC Lichtner, and D Zachmann. 2008. "Science for Problems Under the Surface." *SciDAC Review* 2008(7):32-41.

Schroth M, M Oostrom, R Dobson, and J Zeyer. 2008. "Thermodynamic Model for Fluid/Fluid Interfacial Areas in Porous Media for Arbitrary Drainage/Imbibition Sequences." *Vadose Zone Journal* 7(3):966-971. doi:10.2136/vzj2007.0185

Schuchardt KL, BJ Palmer, JA Daily, TO Elsethagen, and AS Koontz. 2007. "IO Strategies and Data Services for Petascale Data Sets from a Global Cloud Resolving Model." *Journal of Physics: Conference Series* 78:Art. No. 012089 (6pp). doi:10.1088/1742-6596/78/1/012089

Senko JM, SD Kelly, AC Dohnalkova, JT McDonough, KM Kemner, and WD Burgos. 2007. "The Effect of U(VI) Bioreduction Kinetics on Subsequent Reoxidation of Biogenic U(IV)." *Geochimica et Cosmochimica Acta* 71(19):4644-4654. doi:10.1016/j.gca.2007.07.021

Sergeeva AP, DY Zubarev, HJ Zhai, AI Boldyrev, and LS Wang. 2008. "Photoelectron Spectroscopic and Theoretical Study of B-16(-) and B-16(2-): An All-Boron Naphthalene." *Journal of the American Chemical Society* 130(23):7244-7246. doi:10.1021/ja802494z

Shah AR, CS Oehmen, and BJM Webb-Robertson. 2008. "SVM-Hustle - An Iterative Semi-Supervised Machine Learning Approach for Pairwise Protein Remote Homology Detection." *Bioinformatics* 24(6):783-790. doi:10.1093/bioinformatics/btn.028

Shao Y, R Kou, J Wang, VV Viswanathan, JH Kwak, J Liu, Y Wang, and Y Lin. 2008. "The influence of the electrochemical stressing (potential step and potential-static holding) on the degradation of polymer electrolyte membrane fuel cell electrocatalysts." *Journal of Power Sources* 185(1):280-286. doi:10.1016/j.jpowsour.2008.07.008

Sharma A, Y Qiang, DR Meyer, R Souza, A Mcconnaughoy, L Muldoon, and DR Baer. 2008. "Biocompatible core-shell magnetic nanoparticles for cancer treatment." *Journal of Applied Physics* 103(7):Art. No.07A308. doi:10.1063/1.2831791

Shchukarev A, JF Boily, and AR Felmy. 2007. "XPS of Fast-Frozen Hematite Colloids in NaCl Aqueous Solutions: I. Evidence for the Formation of Multiple Layers of Hydrated Sodium and Chloride Ions Induced by the {001} Basal Plane." *Journal of Physical Chemistry C* 111(49):18307-18316. doi:10.1021/jp075321c

Shen Y, KK Hixson, N Tolic, DG Camp, II, SO Purvine, RJ Moore, and RD Smith. 2008. "Mass spectrometry analysis of proteome-wide proteolytic post-translational degradation of proteins." *Analytical Chemistry* 80(15):5819-5828. doi:10.1021/ac800077w

Shen Y, N Tolic, KK Hixson, SO Purvine, L Pasa-Tolic, W Qian, JN Adkins, RJ Moore, and RD Smith. 2008. "Proteome-Wide Identification of Proteins And Their Modifications With Decreased Ambiguities and Improved False Discovery Rates Using Unique Sequence Tags." *Analytical Chemistry* 80(6):1871-82. doi:10.1021/ac702328x

Shi L, S Deng, MJ Marshall, Z Wang, DW Kennedy, A Dohnalkova, HM Mottaz, EA Hill, YA Gorby, AS Beliaev, DJ Richardson, JM Zachara, and JK Fredrickson. 2008. " Direct Involvement of Type II Secretion System in Extracellular Translocation of Shewanella Oneidensis Outer Membrane Cytochromes MtrC and OmcA." *Journal of Bacteriology* 190(15):5512-5516. doi:10.1128/JB.00514-08

Shin Y, IT Bae, BW Arey, and GJ Exarhos. 2008. "Facile stabilization of gold-silver alloy nanoparticles on cellulose nanocrystal." *Journal of Physical Chemistry C* 112(13):4844-4848. doi:10.1021/jp710767w

Shin Y, GA Baker, LQ Wang, and GJ Exarhos. 2008. "Investigation of the hygroscopic growth of self-assembled layers of N-alkyl-N-methylpyrrolidinium bromides at the interface between air and organic salt ." *Colloids and Surfaces. A, Physicochemical and Engineering Aspects* 318(1-3):254-258. doi:10.1016/j.colsurfa.2007.12.045

Shin Y, LQ Wang, IT Bae, BW Arey, and GJ Exarhos. 2008. "Hydrothermal Syntheses of Colloidal Carbon Spheres from Cyclodextrins." *Journal of Physical Chemistry C* 112(37):14236-14240. doi:10.1021/jp801343y

Shukla AK. 2007. "Bimodal Energy Distributions in the Scattering of $Ar^+$ Ions from Modified Surfaces at Hyperthermal Energies." *Chemical Physics Letters* 449(1-3):53-56. doi:10.1016/j.cplett.2007.10.043

Shukla AK. 2007. "Fragmentation Dynamics of CS22+ on Collision with a Self-Assembled Monolayer Surface." *Chemical Physics Letters* 448(4-6):156-158. doi:10.1016/j.cplett.2007.09.083

Sideris PJ, UG Nielsen, Z Gan, and CP Grey. 2008. "Mg/Al Ordering in Layered Double Hydroxides Revealed by Multinuclear NMR Spectroscopy." *Science* 321(5885):113-117. doi:10.1126/science.1157581

Smith MAH, CP Rinsland, TA Blake, RL Sams, DC Benner, and VM Devi. 2008. "Low Temperature Measurements of HCN Broadened by N2 in the 14-micron

Spectral Region." *Journal of Quantitative Spectroscopy and Radiative Transfer* 109(6):922-951. doi:10.1016/j.jqsrt.2007.12.017

Song C, RA Zaveri, ML Alexander, JA Thornton, S Madronich, JV Ortega, A Zelenyuk, X Yu, A Laskin, and DA Maughan. 2007. "Effect of Hydrophobic Primary Organic Aerosols on Secondary Organic Aerosol Formation from Ozonolysis of α-Pinene." *Geophysical Research Letters* 34(20):L20803. doi:10.1029/2007GL030720

Tartakovsky AM, P Meakin, and DM Tartakovsky. 2008. "Stochastic Langevin Model for Flow and Transport in Porous Media." *Physical Review Letters* 101:044502.

Thurber A, KM Reddy, V Shutthanandan, MH Engelhard, C Wang, J Hays, and A Punnoose. 2007. "Ferromagnetism in Chemically Synthesized $CeO_2$ Nanoparticles by Ni Doping." *Physical Review. B, Condensed Matter* 76(16):165206 (p 1-8). doi:10.1103/PhysRevB.76.165206

Toepel J, EA Welsh, T Summerfield, HB Pakrasi, and LA Sherman. 2008. "Differential Transcriptional Analysis of the Cyanobacterium Cyanothece sp. ATCC 51142 during Light-Dark and Continuous-Light Growth." *Journal of Bacteriology* 190(11):3904-3913. doi:10.1128/JB.00206-08

Tolmachev AV, EW Robinson, S Wu, H Kang, NM Lourette, L Pasa-Tolic, and RD Smith. 2008. " Trapped-ion cell with improved DC potential harmonicity for FT-ICR MS." *Journal of the American Society for Mass Spectrometry* 19(4):586 - 597. doi:10.1016/j.jasms.2008.01.006

Tuma J, S Tonzani, GC Schatz, AH Karaba, and FD Lewis. 2007. "Structure and Electronic Spectra of DNA Mini-hairpins with $G_n$:$C_n$ Stems." *Journal of Physical Chemistry B* 111(45):13101-13106. doi:10.1021/jp072303m

Umar AN, M Jaremko, PC Burgers, TM Luider, JA Foekens, and L Pasa-Tolic. 2008. "High-throughput proteomics of breast carcinoma cells: a focus on FTICR-MS." *Expert Review of Proteomics* 2008 Jun;5(3):445-55.

Valiev M, EJ Bylaska, M Dupuis, and PG Tratnyek. 2008. "Combined Quantum Mechanical and Molecular Mechanics Studies of the Electron-Transfer Reactions Involving Carbon Tetrachloride in Solution." *Journal of Physical Chemistry A* 112(12):2713-2720. doi:10.1021/jp7104709

Valiev M, J Yang, JA Adams, SS Taylor, and JH Weare. 2007. "Phosphorylation Reaction in cAPK Protein Kinase-Free Energy Quantum Mechanical/Molecular Mechanics Simulations." *Journal of Physical Chemistry B* 111(47):13455-13464. doi:10.1021/jp074853q
Verrier CLM, JH Kwak, DH Kim, CHF Peden, and J Szanyi. 2008. "NOx uptake on alkaline earth oxides (BaO, MgO, CaO and SrO) supported on γ-Al2O3." *Catalysis Today* 136(1-2):121-127. doi:doi:10.1016/j.cattod.2007.12.138

Walser ML, Y Desyaterik, J Laskin, A Laskin, and SA Nizkorodov. 2008. "High-Resolution Mass Spectrometric Analysis of Secondary Organic Aerosol Produced by

Ozonation of Limonene." *Physical Chemistry Chemical Physics. PCCP* 10(7):1009-1022. doi:10.1039/b712620d

Wan J, TK Tokunaga, Y Kim, Z Wang, A Lanzirotti, E Saiz, and RJ Serne. 2008. "Effect of Saline Waste Solution Infiltration Rates on Uranium Retention and Spatial Distribution in Hanford Sediments." *Environmental Science & Technology* 42(6):1973-1978. doi:10.1021/es070684b

Wang CM, DR Baer, JE Amonette, MH Engelhard, JJ Antony, and Y Qiang. 2007. "Electron Beam-Induced Thickening of the Protective Oxide Layer around Fe Nanoparticles." *Ultramicroscopy* 108(1):43-51. doi:10.1016/j.ultramic.2007.03.002

Wang CM, LV Saraf, TL Hubler, and P Nachimuthu. 2008. "Tilted Domain Growth of Metalorganic Chemical Vapor (MOCVD)-Grown ZnO(0001) on $\alpha$-$Al_2O_3$(0001)." *Journal of Materials Research* 23(1):13-17. doi:10.1557/JMR.2008.0026

Wang D, D Choi, Z Yang, VV Viswanathan, Z Nie, CM Wang, Y Song, J Zhang, and J Liu. 2008. "Synthesis and Li-ion Insertion Properties of Highly Crystalline Mesoporous Rutile TiO2." *Chemistry of Materials* 20(10):3435-3442.

Wang D, and WM Huo. 2008. "An Eight-Degree-of-Freedom, Quantum Dynamics Study of the Isotopic Effect on the Reaction: HD+C   H ." *Journal of Chemical Physics* 129:084303. doi:10.1063/1.2971184

Wang D and WM Huo. 2007. "An Eight-Degree-of-Freedom, Time-Dependent Quantum Dynamics Study for the $H_2$+$C_2H$ Reaction on a New Modified Potential Energy Surface." *Journal of Chemical Physics* 127(15):Art. No. 154304. doi:10.1063/1.2794757

Wang D, Z Ma, S Dai, J Liu, Z Nie, MH Engelhard, Q Huo, CM Wang, and R Kou. 2008. "Low-Temperature Synthesis of Tunable Mesoporous Crystalline Transition Metal Oxides and Applications as Au Catalyst Supports." *Journal of Physical Chemistry C* 112(35):13499-13509. doi:10.1021/jp804250f

Wang H, RC Bell, MJ Iedema, GK Schenter, K Wu, and JP Cowin. 2008. "Pyroelectricity of Water Ice." *Journal of Physical Chemistry B* 112(20):6379-6389. doi:10.1021/jp073870c

Wang J, G Liu, H Wu, and Y Lin. 2008. "Quantum-Dot-Based Electrochemical Immunoassay for High-Throughput Screening of the Prostate-Specific Antigen." *Small* 4(1):82-86. doi:10.1002/smll.200700459

Wang J, G Liu, H Wu, and Y Lin. 2008. "Sensitive electrochemical immunoassay for 2,4,6-trinitrotoluene based on functionalized silica nanoparticle labels." *Analytica Chimica Acta* 610(1):112-118. doi:10.1016/j.aca.2008.01.024

Wang J, and Y Lin. 2008. "Functionalized carbon nanotubes and nanofibers for biosensing applications." *Trends in Analytical Chemistry. TrAC* 27(7):619-626. doi:10.1016/j.trac.2008.05.009

Wang J, C Timchalk, and Y Lin. 2008. "Carbon Nanotube-Based Electrochemical Sensor for Assay of Salivary Cholinesterase Enzyme Activity: An Exposure Biomarker of Organophosphate Pesticides and Nerve Agents." *Environmental Science & Technology* 42(7):2688-2693. doi:10.1021/es702335y

Wang LQ, XD Zhou, GJ Exarhos, LR Pederson, CM Wang, CF Windisch, Jr, and C Yao. 2007. "Proton Dynamics in ZnO Nanorods Quantified by *In Situ* Solid-State $^{1}$H Nuclear Magnetic Resonance Spectroscopy." *Applied Physics Letters* 91(17):Art. No. 173107. doi:10.1063/1.2799734

Wang P, O Hadjar, PL Gassman, and J Laskin. 2008. "Reactive Landing of Peptide Ions on Self-Assembled Monolayer Surfaces: A Alternative Approach for Covalent Immobilization of Peptides on Surfaces." *Physical Chemistry Chemical Physics. PCCP* 10(11):1512-1522. doi:10.1039/b717617a

Wang P, and J Laskin. 2008. "Helical Peptide Arrays on Self-Assembled Monolayer Surfaces through Soft and Reactive Landing of Mass-Selected Ions." *Angewandte Chemie International Edition* 47:6678-6680. doi:10.1002/anie.200801366

Wang XB, J Yang, and LS Wang. 2008. "Observation of Entropic Effect on Conformation Changes of Complex Systems Under Well-Controlled Temperature Condition." *Journal of Physical Chemistry A* 112(2):172-175. doi:10.1021/jp711205z

Wang XB, K Matheis, IN Ioffe, AA Goryunkov, J Yang, MM Kappes, and LS Wang. 2008. "High Resolution and Low-Temperature Photoelectron Spectroscopy of an Oxygen-Linked Fullerene Dimer Dianion: C120O2-." *Journal of Chemical Physics* 128(11):Art. No. 114307.

Wang XB, and LS Wang. 2008. "Development of a Low-Temperature Photoelectron Spectroscopy Instrument Using an Electrospray Ion Source and a Cryogenically Controlled Ion Trap." *Review of Scientific Instruments* 79(7):,

Wang Z, XT Zu, Z Li, and F Gao. 2008. "Amorphous Layer Coating Induced Brittle to Ductile Transition in Single Crystalline SiC Nanowires: An Atomistic Simulation." *Journal of Physics D. Applied Physics* 41(15):155419. doi:10.1088/0022-3727/41/15/155419

Wang Z, XT Zu, L Yang, F Gao, and WJ Weber. 2008. "Buckling of GaN nanotubes under uniaxial compression." *Solid State Communications* 146(7-8):293-297. doi:10.1016/j.ssc.2008.03.004

Wang Z, XT Zu, L Yang, F Gao, and WJ Weber. 2008. "Orientation and Temperature Dependence of the Tensile Behavior of GaN Nanowires: An Atomistic Study." *Journal of Materials Science. Materials in Electronics* 19(8-9):863-867. doi:10.1007/s10854-007-9526-8

Weber WJ, L Wang, Y Zhang, W Jiang, and IT Bae. 2008. "Effects of Dynamic Recovery on Amorphization Kinetics in $^{6}$H-SiC." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 266(12-13):2793-2796. doi:10.1016/j.nimb.2008.03.119

Wellman DM, EM Pierce, and MM Valenta. 2007. "Efficacy of soluble Sodium Tripolyphosphate Amendments for the In-Situ Immobilisation of Uranium." *Environmental Chemistry* 4(5):293-300.

Welsh EA, ML Liberton, J Stockel, T Loh, TR Elvitigala, C Wang, A Wollam, RS Fulton, SW Clifton, JM Jacobs, R Aurora, BK Ghosh, LA Sherman, RD Smith, RK Wilson, and HB Pakrasi. 2008. "The Genome Sequence of *Cyanothece* 51142, a unicellular diazotrophic cyanobacterium important in the marine nitrogen cycle." *Proceedings of the National Academy of Sciences of the United States of America* 105(39):15094-15099. doi:10.1073/pnas.0805418105

White MD, M Oostrom, ML Rockhold, and M Rosing. 2008. "Scalable Modeling of Carbon Tetrachloride Migration in the Deep Vadose Zone at the Hanford Site." *Vadose Zone Journal* 7(2):654-666.

Wigginton NS, KM Rosso, and MF Hochella Jr. 2007. "Mechanisms of Electron Transfer in Two Decaheme Cytochromes from a Metal-Reducing Bacterium." *Journal of Physical Chemistry B* 111(44):12857-12864. doi:10.1021/jp0718698

Wiley HS. 2008. "No to negative data." *The Scientist* 22(4):39.

Wiley HS. 2008. "Telling Science's Stories." *The Scientist* 22(1):27.

Woo BK, W Chen, AG Joly, and R Sammynaiken. 2008. "The Effects of Aging on the Luminescence of PEG-Coated Water-Soluble ZnO Nanoparticles Solutions." *Journal of Physical Chemistry C* 112(37):14292-14296. doi:10.1021/jp803649k

Wu B, A Yee, Y Huang, TA Ramelot, JR Cort, A Semesi, JW Jung, W Lee, MA Kennedy, G Montelione, and CH Arrowsmith. 2008. "The Solution Structure of Ribosomal Protein S17E from Methanobacterium thermoautotrophicum: a Structural Homolog of the FF Domain." *Protein Science* 17(3):583-588.

Wu H, J Wang, Z Wang, DR Fisher, and Y Lin. 2008. "Apoferritin-Templated Yttrium Phosphate Nanoparticle Conjugates for Radioimmunotherapy of Cancers." *Journal of Nanoscience and Nanotechnology* 8(5):2316-2322. doi:10.1166/jnn.2008.177

Wu H, MH Engelhard, J Wang, DR Fisher, and Y Lin. 2008. "Synthesis of Lutetium Phosphate/Apoferritin Core-Shell Nanoparticles for Potential Applications in Radioimmunoimaging and Radioimmunotherapy of Cancers." *Journal of Materials Chemistry* 18(15):1779-1783.

Xiao H, F Gao, LM Wang, XT Zu, Y Zhang, and WJ Weber. 2008. "Structural Phase Transitions in High-Pressure Wurtzite to Rocksalt Phase in GaN and SiC." *Applied Physics Letters* 92(24):Art. No. 241909. doi:10.1063/1.2938724

Xing X, XB Wang, and LS Wang. 2008. "Imaging Intramolecular Coulomb Repulsions in Multiply Charged Anions." *Physical Review Letters* 101(8):Art. no. 083003. doi:10.1103/PhysRevLett.101.083003

Yang F, DG Camp, II, MA Gritsenko, Q Luo, RT Kelly, TRW Clauss, WR Brinkley, RD Smith, and DL Stenoien. 2007. "Identification of a Novel Mitotic Phosphorylation Motif Associated with Protein Localization to the Mitotic Apparatus." *Journal of Cell Science* 120(22):4060-4070. doi:10.1242/jcs.014795
Yang F, N Jaitly, H Jayachandran, Q Lou, ME Monroe, X Du, MA Gritsenko, R Zhang, DJ Anderson, SO Purvine, JN Adkins, RJ Moore, HM Mottaz, S Ding, MS Lipton, DG Camp, II, HR Udseth, RD Smith, and S Rossie. 2007. "Applying a Targeted Label-free Approach using LC-MS AMT Tags to Evaluate Changes in Protein Phosphorylation Following Phosphatase Inhibition." *Journal of Proteome Research* 6(11):4489-4497. doi:10.1021/pr070068e

Yang J, XB Wang, X Xing, and LS Wang. 2008. "Photoelectron Spectroscopy of Anions at 118.2 nm: Observation of High Electron Binding Energies in Superhalogens MCI4- (M=Sc, Y, La)." *Journal of Chemical Physics* 128(20):201102. doi:10.1063/1.2938390

Yang J, X Xing, XB Wang, LS Wang, AP Sergeeva, and AI Boldyrev. 2008. "Negative Electron Binding Energies Observed in a Triply Charged Anion: Photoelectron Spectroscopy of 1-Hydroxy-3, 6, 8-Pyrene-Trisulfonate." *Journal of Chemical Physics* 128(9):Art. No. 091102. doi:10.1063/1.2889001

Yang Z, C Lam, IK Chu, and J Laskin. 2008. "The Effect of the Secondary Structure on Dissociation of Peptide Radical Cations: Fragmentation of Angiotensin III and Its Analogues." *Journal of Physical Chemistry B* 112(39):12468-12478. doi:10.1021/jp805226x

Yang Z, G Xia, MS Walker, CM Wang, JW Stevenson, and P Singh. 2007. "High Temperature Oxidation/Corrosion Behavior of Metals and Alloys Under a Hydrogen Gradient." *International Journal of Hydrogen Energy* 32(16):3770-3777. doi:10.1016/j.ijhydene.2006.08.056

Yanina S, and KM Rosso. 2008. "Linked Reactivity at Mineral-Water Interfaces Through Bulk Crystal Conduction." *Science* 320(5873):218-222. doi:10.1126/science.1154833

Yantasee W, B Charnhattakorn, GE Fryxell, Y Lin, C Timchalk, and RS Addleman. 2008. "Detection of Cd, Pb, and Cu in non-pretreated natural waters and urine with thiol functionalized mesoporous silica and Nafion composite electrodes." *Analytica Chimica Acta* (620):55-63. doi:10.1016/j.aca.2008.05.029

Yantasee W, K Hongsirikarn, CL Warner, D Choi, T Sangvanich, MB Toloczko, MG Warner, GE Fryxell, RS Addleman, and C Timchalk. 2008. "Direct detection of Pb in urine and Cd, Pb, Cu, and Ag in natural waters using electrochemical sensors immobilized with DMSA functionalized magnetic nanoparticles." *The Analyst* 133(3):348-355. doi:10.1039/b711199a

Yantasee W, Y Lin, K Hongsirikarn, GE Fryxell, R Addleman, and C Timchalk. 2007. "Electrochemical Sensors for the Detection of Lead and Other Toxic Heavy Metals: The Next Generation of Personal Exposure Biomonitors." *Environmental Health Perspectives* 115(12):1683-1690.

Yao C, Y Shin, LQ Wang, CF Windisch, JR, WD Samuels, BW Arey, CM Wang, WM Risen Jr., and GJ Exarhos. 2007. "Hydrothermal Dehydration of Aqueous Fructose Solutions in a Closed System." *Journal of Physical Chemistry C* 111(42):15141-15145. doi:10.1021/jp074188l

Yi CW and J Szanyi. 2007. "$D_2O$ Adsorption on an Ultrathin Alumina Film on NiAl(110)." *Journal of Physical Chemistry C* 111(47):17597-17602. doi:10.1021/jp074459s

Yi CW, JH Kwak, and J Szanyi. 2007. "Interaction of $NO_2$ with BaO: From Cooperative Adsorption to $Ba(NO_3)_2$ Formation." *Journal of Physical Chemistry C* 111(42):15299-15305. doi:10.1021/jp074179c

Yi CW, JH Kwak, CHF Peden, CM Wang, and J Szanyi. 2007. "Understanding Practical Catalysts Using a Surface Science Approach: The Importance of Strong Interaction between BaO and $Al_2O_3$ in $NO_x$ Storage Materials." *Journal of Physical Chemistry C* 111(41):14942-14944. doi:10.1021/jp0763376

Yoon H, C Werth, AJ Valocchi, and M Oostrom. 2008. "Impact of Nonaqueous Phase Liquid (NAPL) Source Zone Architecture on Mass Removal Mechanisms in Strongly Layered Heterogeneous Porous Media during Soil Vapor Extraction." *Journal of Contaminant Hydrology* 100(1-2):58-71. doi:10.1016/j.jconhyd.2008.05.006

Yu Y, MJ Ezell, AN Zelenyuk, DG Imre, ML Alexander, JV Ortega, B D'Anna, CW Harmon, S Johnson, and BJ Finlayson-Pitts. 2008. "Photooxidation of Alpha-Pinene at High Relative Humidity in the Presence of Increasing Concentrations of NOx." *Atmospheric Environment* 42(20):5044-5060.

Yu Y, MJ Ezell, AN Zelenyuk, DG Imre, ML Alexander, JV Ortega, JL Thomas, K Gogna, DJ Tobias, B D'Anna, CW Harmon, S Johnson, and BJ Finlayson-Pitts. 2008. "Nitrate Ion Photochemistry at Interfaces: A New Mechanism for Oxidation of alpha-Pinene." *Physical Chemistry Chemical Physics. PCCP* 10(21):3063-3071. doi:10.1039/b719495a

Yu ZQ, SVNT Kuchibhatla, MH Engelhard, V Shutthanandan, CM Wang, P Nachimuthu, OA Marina, LV Sara, S Thevuthasan, and S Seal. 2008. "Growth and Structure of Epitaxial $Ce_{0.8}Sm_{0.2}O_{1.9}$ by Oxygen-Plasma-Assisted Molecular Beam Epitaxy." *Journal of Crystal Growth* 310(10):2450-2456. doi:10.1016/j.jcrysgro.2007.12.028

Yu Z, S Kuchibhatla, LV Saraf, OA Marina, CM Wang, MH Engelhard, V Shutthanandan, P Nachimuthu, and S Thevuthasan. 2008. "Conductivity of Oriented Samaria-Doped Ceria Thin Films Grown by Oxygen-plasma-assisted Molecular Beam Epitaxy." *Electrochemical and Solid-State Letters* 11(5):B76-B78. doi:10.1149/1.2890122

Zehr RT, and MA Henderson. 2008. "Acetaldehyde Photochemistry on $TiO_2(110)$." *Surface Science* 602(13):2238-2249. doi:10.1016/j.susc.2008.04.045

Zelenyuk AN, DG Imre, J Han, and S Oatis. 2008. "Simultaneous Measurements of Individual Ambient Particles Size, Composition, Effective Density, and Hygroscopicity." *Analytical Chemistry* 80(5):1401-1407. doi:10.1021/ac701723v

Zelenyuk AN, DG Imre, EJ Nam, Y Han, and K Mueller. 2008. "ClusterSculptor: Software for Expert-Steered Classification of Single Particle Mass Spectra." *International Journal of Mass Spectrometry* 275(1-3):1-10. doi:10.1016/j.ijms.2008.04.033

Zelenyuk AN, J Yang, C Song, RA Zaveri, and DG Imre. 2008. ""Depth-Profiling" and Quantitative Characterization of the Size, Composition, Shape, Density, and Morphology of Fine Particles with SPLAT, a Single-Particle Mass Spectrometer." *Journal of Physical Chemistry A* 112(4):669-677. doi:10.1021/jp077308y

Zhai HJ, C Burgel, V Bonacic-Koutecky, and LS Wang. 2008. "Probing the Electronic Structure and Chemical Bonding of Gold Oxides and Sulfides in AuOn- and AuSn- (n=1, 2)." *Journal of the American Chemical Society* 130(28):9156-9167. doi:10.1021/ja802408b

Zhai HJ, J Döbler, J Sauer, and LS Wang. 2007. "Probing the Electronic Structure of Early Transition-Metal Oxide Clusters: Polyhedral Cages of $(V_2O_5)_n^-$ ($n$=2-4) and $(M_2O_5)_2^-$ (M=Nb, Ta)." *Journal of the American Chemical Society* 129(43):13270-13276. doi:10.1021/ja0750874

Zhai HJ, S Li, DA Dixon, and LS Wang. 2008. "Probing the Electronic and Structural Properties of Chromium Oxide Clusters (CrO3)n- and (CrO3)n (n=1-5): Photoelectron Spectroscopy and Density Functional Calculations." *Journal of the American Chemical Society* 130(15):5167-5177.

Zhai HJ, LL Pan, B Dai, B Kiran, J Li, and LS Wang. 2008. "Chemisorption-Induced Structural Changes and Transition from Chemisorption to Physisorption in Au6(CO)n-(n=4-9)." *Journal of Physical Chemistry C* 112(31):11920-11928. doi:10.1021/jp803161b

Zhang H, X Tang, GR Munske, NL Zakharova, L Yang, C Zheng, MA Wolff, N Tolic, GA Anderson, L Shi, MJ Marshall, JK Fredrickson, and JE Bruce. 2008. "In Vivo Identification of the Outer Membrane Protein OmcA-MtrC Interaction Network in Shewanella oneidensis MR-1 Cells Using Novel Hydrophobic Chemical Cross-Linkers." *Journal of Proteome Research* 7(4):1712-1720. doi:10.1021/pr7007658

Zhang M, LA Boatner, E Salje, RC Ewing, P Daniel, WJ Weber, Y Zhang, and I Farnan. 2008. "Micro-Raman and Micro-Infrared Spectroscopic Studies of Pb- and Au-Irradiated ZrSiO4: Optical Properties, Structural Damage and Amorphization ." *Physical Review. B, Condensed Matter and Materials Physics* 77(14):144110. doi:10.1103/PhysRevB.77.144110

Zhang Q, YJ Shing, F Hua, LV Saraf, and DW Matson. 2008. "Fabrication of Transparent Capacitive Structure by Self-Assembled Thin Films." *Journal of Nanoscience and Nanotechnology* 8(6):3008-3012.

Zhang Y, IT Bae, and WJ Weber. 2008. "Atomic Collision and Ionization Effects in Oxides." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 266(12-13):2828-2833. doi:10.1016/j.nimb.2008.03.197

Zhang Y, M Elfman, BD Milbrath, and WJ Weber. 2008. "Evaluate Scintillation Response Over a Continuous Energy Region." *IEEE Transactions on Nuclear Science* 55(3):1097-1101. doi:10.1109/TNS.2008.922821

Zhang Y, X Xiang, and WJ Weber. 2008. "Scintillation Response of CaF2 to H and He over a Continuous Energy Range." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 266(12-13):2750-2753. doi:10.1016/j.nimb.2008.03.110

Zheng H, D Ma, X Bao, JZ Hu, JH Kwak, Y Wang, and CHF Peden. 2008. "Direct Observation of the Active Center for Methane Dehydroaromatization Using an Ultrahigh Field 95Mo NMR Spectroscopy." *Journal of the American Chemical Society* 130(12):3722-3723. doi:10.1021/ja7110916

Zhong L, M Oostrom, TW Wietsma, and MA Covert. 2008. "Enhanced Remedial Amendment Delivery through Fluid Viscosity Modifications: Experiments and numerical simulations." *Journal of Contaminant Hydrology* 101(1-4):29-41. doi:10.1016/j.jconhyd.2008.07.007

Zhu M, J Wang, BC Holloway, RA Outlaw, X Zhao, K Hou, V Shutthanandan, and DM Manos. 2007. "A Mechanism for Carbon Nanosheet Formation." *Carbon* 45(11):2229-2234. doi:10.1016/j.carbon.2007.06.017

Zubarev DY, BB Averkiev, HJ Zhai, LS Wang, and AI Boldyrev. 2008. "Aromaticity and Antiaromaticity in Transition-Metal Systems." *Physical Chemistry Chemical Physics. PCCP* 10(2):257-267. doi:10.1039/b713646c

Zubkov T, RS Smith, TR Engstrom, and BD Kay. 2007. "Adsorption, Desorption, and Diffusion of Nitrogen in a Model Nanoporous Material. I. Surface Limited Desorption Kinetics in Amorphous Solid Water." *Journal of Chemical Physics* 127(18):Art. No. 184707. doi:10.1063/1.2790432

**Book Chapter**

Bigelow DJ and W Qian. 2008. "Quantitative Proteome Mapping of Nitrotyrosines." In *Methods in Enzymology, Nitric Oxide Part F: Oxidative and Nitrosative Stress in Redox Regulation of Cell Signaling*, vol. 440, pp. 191-205. Elsevier, Amsterdam, Netherlands. doi:10.1016/S0076-6879(08=7)00811-7

Chen G, and Y Lin. 2008. " Electrochemical Techniques." In *Encyclopedia of Microfluidics and Nanofluidics*, ed. D. Li, pp. 469-474. Springer, Berlin Heidelberg New York , Germany.

Deutsch WJ. 2008. "Contaminant Release from Residual Waste in Closed Single-Shell Tanks and Other Waste Forms Associated with the Tanks." Chapter 19 in *The*

*Resource Conservation and Recovery Act Facility Investigation (RFI) Report for Hanford Single-Shell Tank Waste Management Areas, DOE/ORP-2008-01 Revision 0*, vol. Tier 1, ed. FM Mann, pp. 19-1 - 19-14. U.S. Department of Energy, Office of River Protection, Richland, WA.

Deutsch WJ, KJ Cantrell, RJ Serne, and EM Pierce. 2008. "Appendix D: Contaminant Release from Residual Waste in Closed Single Shell Tanks and Other Waste Forms Associated with the Tanks." In *The Resource Conservation and Recovery Act Facility Investigation (RFI) Report for Hanford Single-Shell Tank Waste Management Areas, DOE/ORP-2008-01 Revision 0*, vol. Tier 2, ed. FM Mann. U.S. Department of Energy, Office of River Protection, Richland, WA.

Fayer MJ, and JM Keller. 2008. "Appendix C: Recharge." In *The Resource Conservation and Recovery Act Facility Investigation (RFI) Report for Hanford Single-Shell Tank Waste Management Areas, DOE/ORP-2008-01 Revision 0*, vol. Tier 2, ed. FM Mann. U.S. Department of Energy, Office of River Protection, Richland, WA.

Liu G, J Wang, Y Lin, and J Wang. 2007. "Nanoparticle-Based Biosensors and Bioassays." Chapter 14 in *Electrochemical Sensors, Biosensors and their Biomedical Applications*, ed. X. Zhang, H. Ju, J. Wang, pp. 441-457. Academic Press, Burlington, MA.

Wang J, G Liu, and Y Lin. 2008. "Layer-by-Layer Assembly of Enzymes on Carbon Nanotubes." Chapter 6 in *Biomolecular Catalysis Nanoscale Science and Technology*, vol. ACS Symposium Series 986, ed. J. Kim, S. H. Kim, P. Wang, pp. 117-128. American Chemical Society, Washington DC.