EMSL Quarterly Highlights Report

3rd Quarter, Fiscal Year 2008

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

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

Research Highlights

Atmospheric Aerosol Chemistry

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.

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.

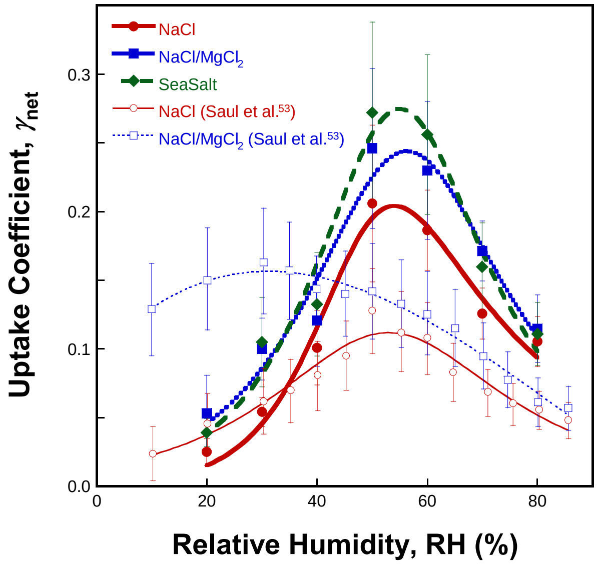

Figure 1. *Values of uptake coefficient as a function of relative humidity for HNO_3 reaction with an NaCl, mixture of NaCl/$MgCl_2$ and sea salt particles (Liu et al, 2007).*

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*.

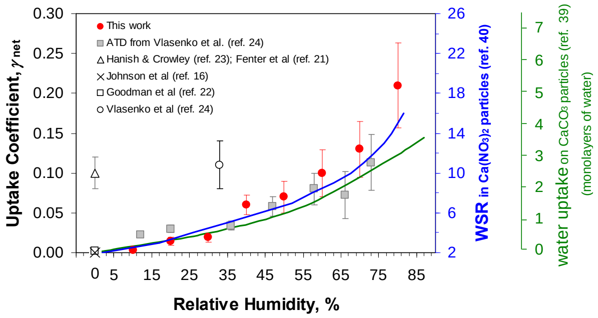

Figure 2. *Experimentally determined uptake coefficient as a function of the relative humidity for HNO_3 reaction with $CaCO_3$ particles (Liu et al. 2008).*

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.

Biological Interactions and Dynamics

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 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.

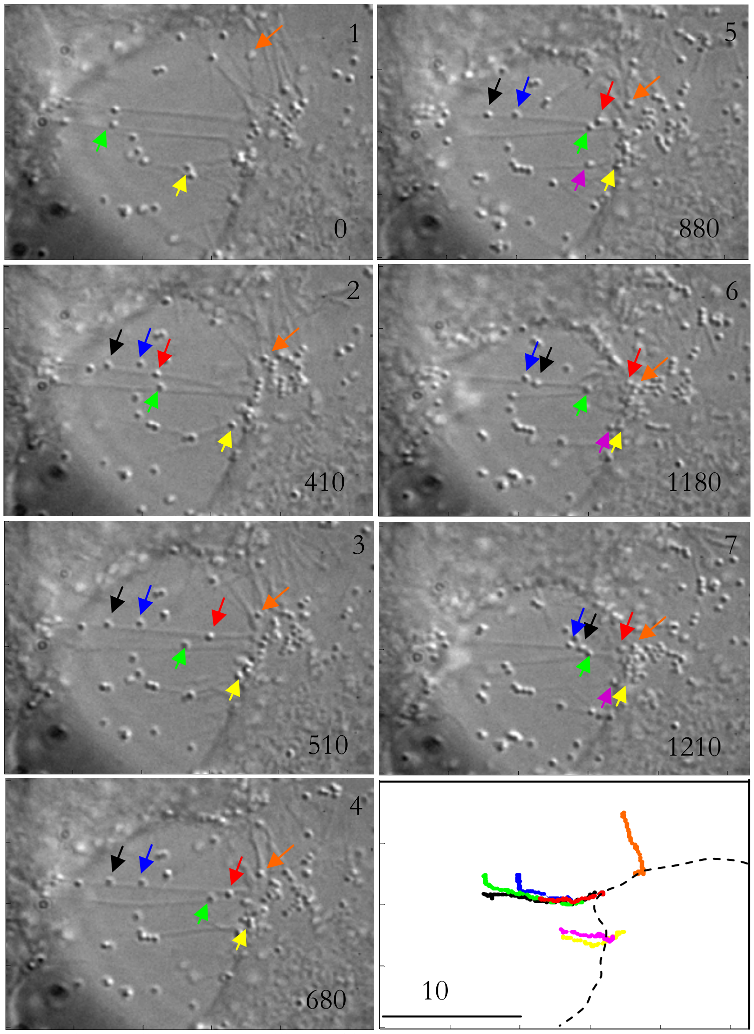

Figure 1. *The retrograde motion unravels the coupling of the particles with the intracellular environment across the cell membrane.*

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.

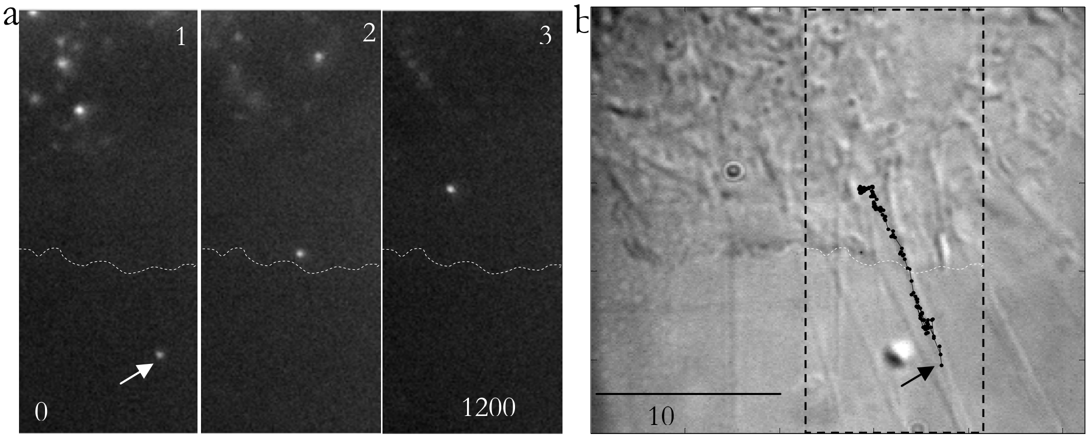

***Figure 2.** The retrograde motion of 100-nm particles using single-molecule fluorescence techniques.*

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.

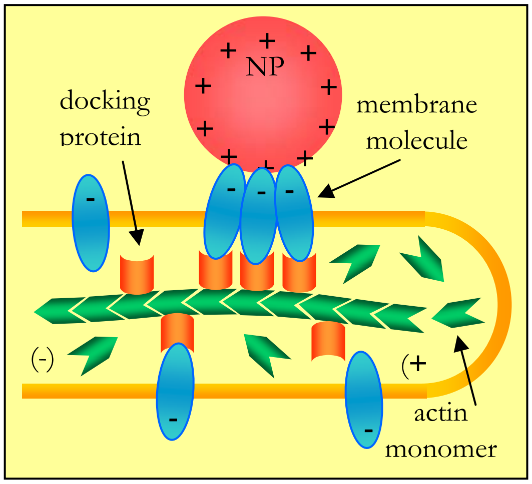

***Figure 3.** Researchers found that the actin treadmilling powers the retrograde motion of the particles.*

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.

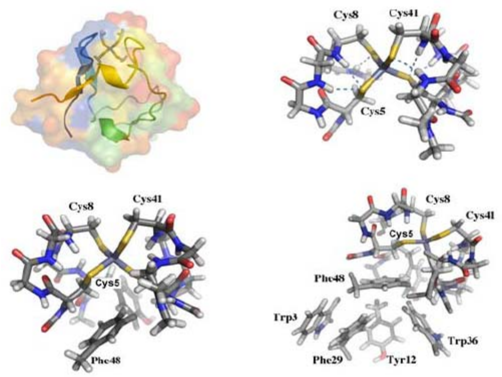

Figure 1. *Structure of the zinc- and cysteine-containing region of* Pyrococcus furiosis *rubredoxin determined with different computational chemistry models.*

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.

Geochemistry/Biogeochemistry and Subsurface Science

None reported during this quarter.

Science of Interfacial Phenomena

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.

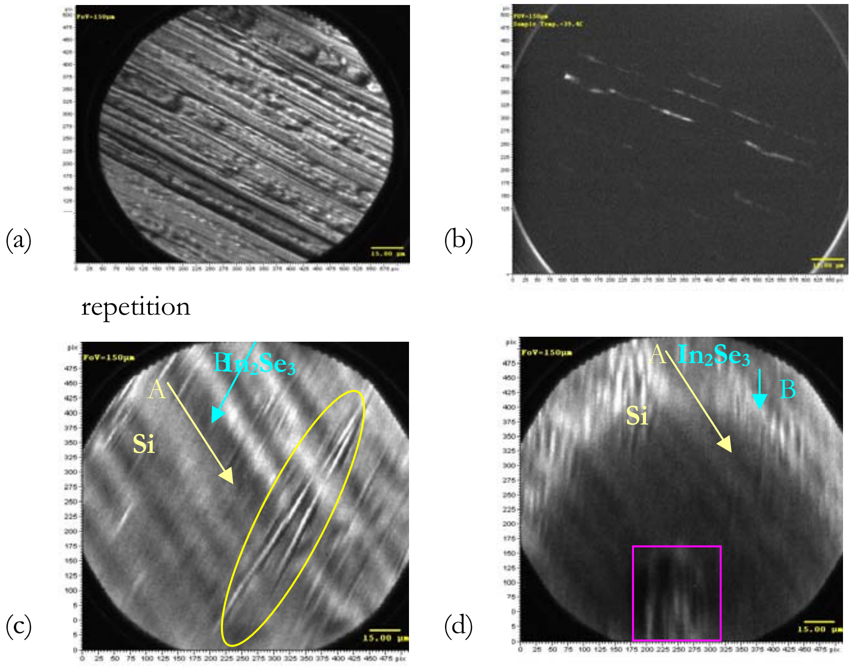

Figure 1. *PEEM images (field of view 150 μm, scale bar 30 μm) for (a) clean Si(111); (b) amorphous In_2Se_3 film on Si(111); (c) annealed In_2Se_3/Si(111); (d) after irradiation with 266-nm photon pulse. Images presented here are acquired with mercury lamp illumination (hν = 5.1 eV).*

The EMSL PEEM was equipped with both Hg (hν = 5.1 eV) and D_2 (hν = 6.0 eV) sources for imaging a 150-μm-diameter region of the sample. An Nd:YAG laser (λ = 266 nm, hν = 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(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/cm². 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.

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 μ_B/Co to >6 μ_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.

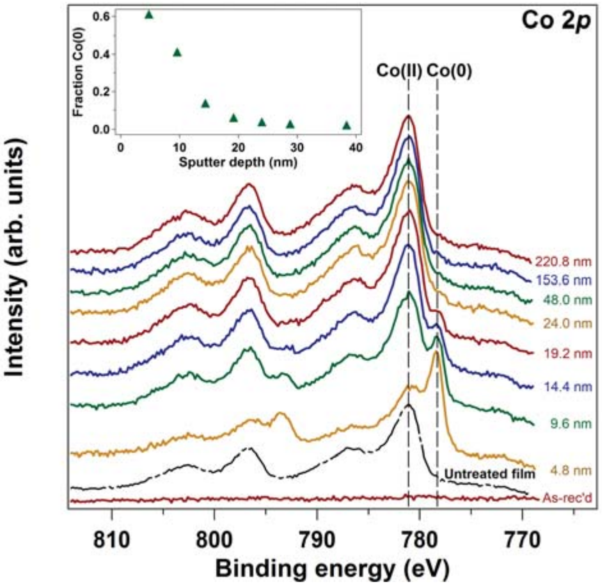

Figure 1. *X-ray photoelectron spectroscopy depth profiles of 310 nm a-$Co_{0.1}Zn_{0.9}O$ after zinc treatment. For comparison, the cobalt 2p spectrum of an untreated film after one sputter cycle is shown (dash-dot line). Inset: fraction of cobalt present as Co(0) as a function of depth in Zn_i:Co:ZnO,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

Weak ferromagnetism in Co:ZnO (0.1 – 0.3 μ_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 μ_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.

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].

Citations:
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.

A Fast Analysis Technique to Evaluate Scintillation Response

***Y Zhang*[(a)]*, M Elfman*[(b)]*, BD Milbrath,*[(c)] *and WJ Weber*[(c)]**
(a) EMSL, Richland, Washingto
(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

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.

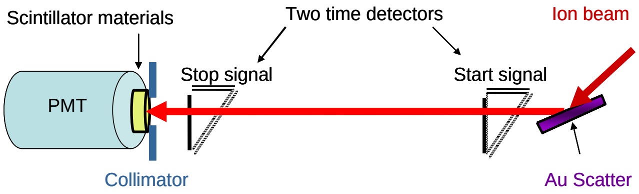

Figure 1. *Schematic drawing of the TOF-scintillator-PMT setup for the scintillation measurement, where BGO or CaF_2:Eu is mounted between the second time detector and the PMT.*

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.

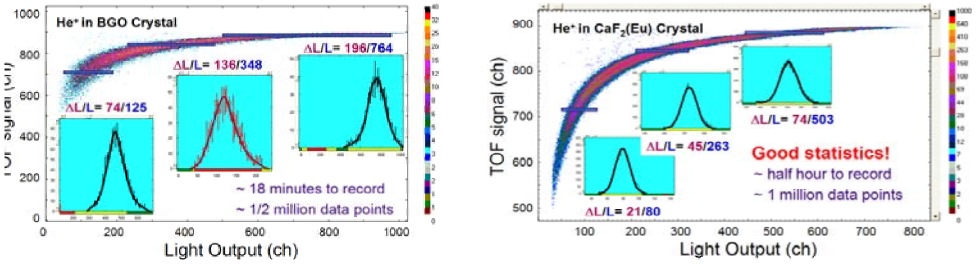

***Figure 2**. TOF versus light output of BGO (left) and CaF_2:Eu (right) to He^+ particles. The insets are the light output profile of the particle at TOF=715, 840 and 885, respectively. The light intensity is governed by the peak position L and the energy resolution can be determined by ΔL/L as shown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

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 ($\Delta L/L$). Fast determination of energy resolution of scintillation response can be obtained by online analysis, as shown by the three examples with corresponding $\Delta L/L$ 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).

TABLE I

FAST ESTIMATION OF ENERGY RESOLUTION ($\Delta L/L$) OF SCINTILLATION RESPONSE

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

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).

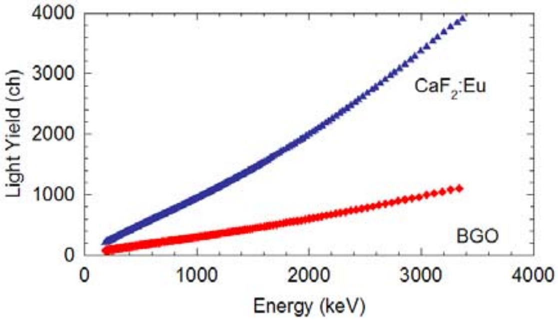

Figure 3. *Light yield (L) as a function of particle energy (E) for CaF_2:Eu and BGO from a similar experimental setup.*

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.

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

ZnO is a wide-bandgap semiconductor material with wide application in the field of optoelectronics, spintronics, piezoelectric transducers, and ultraviolet optoelectronics (Fan and Liu 2005). Considerable research effort has been made for modifying the properties of the ZnO through tailoring of the structure of the material, typically such as doping, grown ZnO into different dimensional structures (dots, thin film, and bulk materials). One of most useful forms of ZnO is the thin film. The key challenge for growing ZnO into a thin film is the control of defect structure in the film, because defects influence the optical and electrical properties of the film. Selection of the substrate and the control of the defect across the interface between the substrate and the film play an important role on the quality of the grown film. This research addresses the defect structure of the ZnO thin film grown on a sapphire substrate.

ZnO grown on (0001) sapphire will generally be oriented such that α-Al_2O_3 (0001)//ZnO(0001). Variable in-plane orientation may lead to two domains such that: α -Al_2O_3 [11-20]//ZnO[11-20] and α -Al_2O_3 [11-20]//ZnO[10-10]. The first mode corresponds to the hexagon-on-hexagon growth and the second mode corresponds to a 30-degree in-plane rotation of the ZnO relative to the α -Al_2O_3. Since it is difficult to obtain an ideal sapphire surface with a well-defined surface structure, various rotation domains, such as the 30-degree rotation domains and a recently reported 21.8-degree rotation domain, may coexist. A previous study shows that by using gallium pre-deposition to modify the sapphire (0001) surface, rotated domains can be completely eliminated. Another growth parameter that could be controlled is the selection of the orientation of the substrate. It has been generally realized that ZnO grown on r-cut sapphire possesses a high quality. However, there is no direct comparison of the film quality grown on both r-cut and c-plane oriented sapphire under an identical growth condition.

In this paper, we report a comparison of the structural features of ZnO thin films grown on both r-cut and c-plane sapphire using metal organic chemical vapor deposition (MOCVD) under identical growth conditions (Wang et al. 2008). It has been found that the film grown on r-cut sapphire shows high-quality single crystals. Film grown on the c-plane shows a range of domains, one that corresponds to the classic growth mode. At the same time, a new growth mode was observed following the deposition of ZnO thin film on α -Al_2O_3 (0001). In this new growth mode, α -Al_2O_3 [11-20]//ZnO[10-10], but the (0001) plane of ZnO is tilted relative to the (0001) plane of α -Al_2O_3 such that ZnO(0001) is almost parallel to the α -Al_2O_3 (-1104) plane.

Growth of the film was performed using a three-source EMCORE MOCVD reactor. The precursor preparation was done by dissolving $Zn(C_{11}H_{19}O_2)_2$-Bis(2,2,6,6-tetramethyl-3,5-heptanedionato) zinc powder in tetrahydrofuran at a concentration of 0.025 M. During the depositions, the substrates were rotated at 500 rpm and the substrate temperature was varied between 450 ºC to 600 ºC. The carrier gas pressure during the growth was kept at 0.28 MPa with a zinc precursor flow rate of 100 g/hr. The operating pressure was kept at 10 Torr with a mixed gases of oxygen and argon flows of 500 sccm and 2000 sccm, respectively. Single crystals of α -Al_2O_3 (0001) and r-cut α -Al_2O_3 were used as substrates.

The film grown on r-cut α -Al_2O_3 possesses a single orientation with respect to the substrate. The interface shows some contrast features that are related to the mismatch dislocations. This feature is further revealed by the high-resolution transmission electron microscopy image illustrated in Figure 1. The interface was featured by very high density of misfit dislocations. The dislocation is not evenly distanced along the interface. Rather, it appears that the dislocation is coupled, leading to a pattern of two dislocations forming a pair. The physical reason for this must be studied. Across the interface, on average, every sixth of α -Al_2O_3 (-12-10) plane terminates at the interface. This result is consistent with that when the film grown on the α -Al_2O_3 (0001) plane. However, the dislocation appears to be uniformly distributed when grown on the (0001) direction. Using the α -Al_2O_3 (-12-10) lattice plane space of 2.3794 Å as an internal standard, the ZnO (01-10) lattice plane space was determined to be 2.773 Å. This will lead to a lattice constant for ZnO to be 3.202 Å, which is slightly smaller than the literature data of 3.249 Å.

ZnO films grown by MOCVD on α -Al_2O_3 (0001) using the Zn $(TMHD)_2$ precursor show granular structures and the grains possess different orientations. Based on electron diffraction and high-resolution transmission electron microscopy imaging, at least two distinct orientations have been identified. One corresponds to the classic 30-degree in-plane rotational domain. The other also includes the 30-degree rotational domain, but, instead of the ZnO (0001) plane being parallel to the (0001) plane of α -Al_2O_3, the (0001) plane of ZnO is tilted ~ 38-degrees in such a way that the (0001) plane of ZnO is approximately parallel with the (-1104) plane of α -Al_2O_3. This tilting of the (0001) plane results in a reduction of interface lattice mismatch from ~18 percent to ~ 2 percent in one direction. Therefore, the tilted growth mode was driven by minimization of interfacial energy. The film grown on r-cut α -Al_2O_3 showed a single crystalline structure and the interface was featured by a high density of mismatch dislocations.

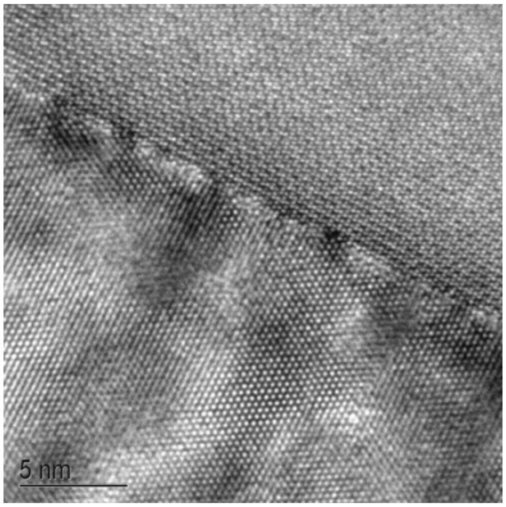

Figure 1. *High-resolution transmission electron microscopy image showing the interface between α -Al_2O_3 and ZnO with the film grown on r-cut α -Al_2O_3.*

Citations

Fan Z, and JG Lu. 2005. "Zinc Oxide Nanostructures: Synthesis and Properties." *Journal of Nanoscience and Nanotechnology* 5(12):1561-1573.

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 MaterialsResearch* 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.

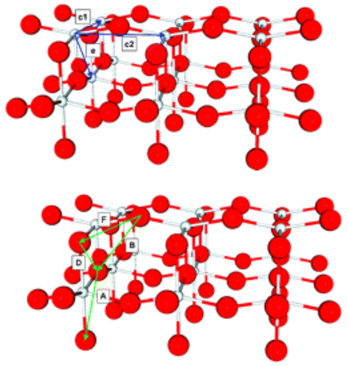

Figure 1. *Electron (top) and hole (bottom) polaron transfer directions at the anatase (001) surfaces.*

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.

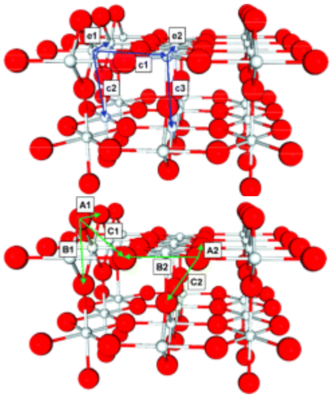

Figure 2. *Electron (top) and hole (bottom) polaron transfer directions at the rutile (110) surface.*

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.

Citations

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.

Major Upgrades

Chinook installation. Phase I of the new supercomputer, Chinook, has been installed and user migration has begun.

News Coverage

Rob Farber was interviewed by the Texas Advanced Computing Center for a feature article that should appear on their web site (http://www.tacc.utexas.edu) in July.

Awards and Recognition

EMSL User receives M.T. Thomas Award for Postdoctoral Accomplishments. EMSL user **Zhenrong Zhang** (Pacific Northwest National Laboratory) was selected as the 2007 recipient EMSL's 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. She 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. At EMSL, Zhang designed a new sample heating stage and implemented a breakthrough methodology that resulted in near-perfect TiO_2 surfaces with negligible water contamination. Her methodology was the crucial advance needed to identify the preferred adsorption or adherence sites and dissociation pathways for water and alcohols as well as the diffusion dynamics of surface defects and hydroxyl groups.

EMSL User receives Biemann Medal. EMSL researcher Julia Laskin (Pacific Northwest National Laboratory) 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 in Denver. The award recognizes Laskin's contributions to better understanding the activation, fragmentation and deposition of large molecules when they collide with surfaces.

Visitors and Users

During the third quarter of Fiscal Year 2008, a total of 380 users benefited from EMSL capabilities and expertise. This total included 289 onsite users and 101 remote users.

New EMSL Staff

Brock Erwin and Jimmy Wanner of WSU Tri-Cities joined EMSL as summer interns.

Publications

Book Chapters

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.

Journal Articles

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

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

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 .

Bowers GM, DL Bish, and RJ Kirkpatrick. 2008. "H2O and Cation Structure and Dynamics in Expandable Clays: 2H and 39K NMR Investigations of Hectorite." *Journal of Physical Chemistry C* 112(16):6430-6438. doi:10.1021/jp7119087

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 (η2) 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, 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* 2:25-28.

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, 13C, and 15N 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.

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.

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

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

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.

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

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, CHF Peden, and J Szanyi. 2008. "Carbonate Formation and Stability on a Pt/BaO/γ-Al2O3 NOx Storage/Reduction Catalyst." *Journal of Physical Chemistry C* 112(29):10952-10959. doi:10.1021/jp712180q

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.

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

Fredrickson JK, and JM Zachara. 2008. "Electron Transfer at the Microbe-Mineral Interface: A Grand Challenge in Biogeochemistry." *Geobiology* 6(3):245-253.

Gardner JS, E Shurdha, CM Wang, LD Lau, RG Rodriguez, and JJ Pak. 2008. "Rapid Synthesis and Size Control of CuInS2 Semi-Conductor Nanoparticles Using Microwave Irradiation." *Journal of Nanoparticle Research* 10(4):633-641. doi:10.1007/s11051-007-9294-7

Gardner JS, E Shurdha, CM Wang, LD Lau, RG Rodriguez, and JJ Pak. 2008. "Rapid synthesis and size control of CuInS2 semi-conductor nanoparticles using microwave irradiation." *Journal of Nanoparticle Research* 10(4):633-641.

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.

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, 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

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

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

Henderson MA. 2008. "Effect of Coadsorbed Water on the Photodecomposition of Acetone on TiO2(110)." *Journal of Catalysis* 256(2):287-292. doi:10.1016/j.jcat.2008.03.020

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

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, 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

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.

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

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 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.

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, 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

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.

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, 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.

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

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

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

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.

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

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

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

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

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

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

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

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

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

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, 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

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

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

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.

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 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, 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 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

Weber WJ, L Wang, Y Zhang, W Jiang, and IT Bae. 2008. "Effects of dynamic recovery on amorphization kinetics in 6H-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

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.

Wiley HS. 2008. "No to negative data." *The Scientist* 22(4):39.

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

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

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

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.

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.

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

Conferences and Presentations

During the third quarter of Fiscal Year 2008, EMSL staff and users presented on research performed at the user facility or attended conferences at the following meetings or locations:

- 2nd On-Line Particle Mass Spectrometry Workshop, Leeds, United Kingdom, April 9, 2008
- 25th Rare Earth Research Conference, Tuscaloosa, Alabama, June 22-29, 2008
- 213th Electro Chemical Society Conference, Phoenix, Arizona, May 22, 2008
- 235th ACS National Meeting, New Orleans, Louisiana, April 7, 2008

- 2008 Symposium on Radiation Measurements and Applications, Berkeley, California, June 2, 2008
- American Ceramic Society 2008 Glass & Optical Materials Division Meeting, Tucson, Arizona, May 19, 2008
- American Society for Mass Spectrometry Conference, Denver, Colorado, June 1-5, 2008
- DICE Workshop, Mason Ohio, May 6, 2008
- DOE Office of Basic Energy Sciences Principal Investigator Meeting, Richland, Washington, June 11, 2008
- High School Student Research Internship, Richland, Washington, May 22, 2008
- HP-CAST meeting, Singapore, May 21, 2008
- International Symposium on Molecular Spectroscopy, Columbus, Ohio, June 15-20, 2008
- LDRD-RDMD Review, Richland, Washington, June 24, 2008
- LinuxFest Northwest 2008, Bellingham, Washington, April 26, 2008
- NSTI Nanotech 2008, Boston, Massachussets, June 4, 2008
- Teragrid 2008, Las Vegas, Nevada, June 10, 2008