

**EMSL Report**  
**May/June 2004**

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## Research Highlights

### Removal of DNAPL from a Layered Porous Medium by Means of Vapor Extraction Enhanced by Desiccation and Water Table Reduction

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Vapor extraction is an *in situ* soil-cleaning process designed to remove volatile organic compounds (VOCs) from the unsaturated (vadose) zone of soil. Some of the more commonly occurring VOCs that have contaminated soil and ground water are the dense non-aqueous phase liquids (DNAPLs) trichloroethylene, perchloroethylene, and carbon tetrachloride (CCl<sub>4</sub>). These contaminants can occur in the liquid phase as free, residual, and/or trapped; in the solid phase by means of adsorption, especially to organic matter; in the aqueous phase when dissolved; and/or in the gas phase.



**Figure 1.** The four sloping layers from top to bottom consisted of a fine, a coarse, a fine, and a coarse material. The initial simulated DNAPL spill is the red sphere.

Any remediation treatment stands to benefit from a proper analysis of the liquid and gaseous flow regimes and their fate in the subsurface environment. The model must, however, give a true description of all physical, chemical, and biological phenomena. There is a need, therefore, to continuously test models by comparing their results with quantitative data obtained during controlled experiments that mimic real situations. Based on some of our knowledge gaps and desire to enhance our understanding of DNAPL fate in the environment and subsequent cleanup activities, we formulated the following objectives:

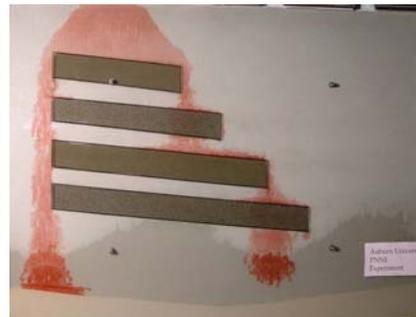
- Investigate the infiltration and redistribution of a DNAPL in a variably saturated, layered porous medium by means of an intermediate-scale experiment.
- Remove the non-trapped DNAPL present in the vadose zone by means of wet vapor extraction.
- Remove trapped DNAPL from the vadose zone and that present in the saturated zone by reducing the water table level and dry vapor extraction.
- Model the processes of the first three objectives using STOMP (Subsurface Transport Over Multiple Phases) and compare numerical and experimental results.

To perform the experimental part, four sloped layers were embedded in an otherwise mainly homogeneous porous medium. From top to bottom, these layers consisted of a fine, a coarse, a fine, and a coarse material (Figure 1). The purpose of this layering was to obtain a clear picture of DNAPL behavior at sloped interfaces of materials with different pore sizes and consequently with different hydraulic properties, like permeability and displacement pressures. The layers were also thought to affect any remediation efforts. To mimic a real situation, the materials for the layers were obtained from the Hanford Site in Richland, Washington.

Figures 1 through 4 show a series of four time-elapsing photos taken of the experiment. Initially (Figure 1), the DNAPL infiltrated very much as a sphere, similarly to the infiltration of water from a point source into dry soil. Once the DNAPL reached the first fine layer, it started to spread to the left and to the right and edged over both ends (Figure 2). During the subsequent redistribution, the DNAPL continued to move straight downward on the left side of the flow cell (high ends of the layers), but followed a more intriguing path at the lower ends. The first coarse layer, which was unsaturated, accepted the DNAPL after some spreading occurred at the boundary, again indicating that the DNAPL moved as a wetting fluid in the unsaturated zone. Once it had entered the first coarse layer, the DNAPL moved straight downward (Figure 2), a result of the diminished capillary action of the bigger pores. As time progressed, the DNAPL on the left side had reached the capillary fringe (saturated zone) and apparently was under enough pressure to displace the water



**Figure 2.** Once the DNAPL reached the first fine layer, it started to spread to the left and right and edged over both ends. When the DNAPL hit the coarse material (second layer) on the right, the solution moved through it.



**Figure 3.** On the right side, the DNAPL continues to move downwards in a stair step pattern: spreading across the fine material then down, moving through the coarse material, spreading across the fine material then down, and then moving through the final coarse material. The collapse of the capillary fringe was evident on both the right and left sides near the DNAPL.

(Figure 3). Meanwhile, on the right side of the layers, the free DNAPL had moved through the coarse layer, accumulated on top of the second fine layer, and started to flow down the boundary until it spilled over the edge (Figure 3). It then started to spread somewhat on top of and move into the second coarse layer (unsaturated).

As with the first coarse layer, the DNAPL moved subsequently straight through and entered the underlying finer material without much delay. The DNAPL again affected the surface tension of water, because the capillary fringe on the right side had also started to collapse (Figure 3). The final DNAPL distribution, for which we assumed static equilibrium, is shown in Figure 4. It clearly shows the collapse of the capillary fringe, which was attributed to a reduction of the surface tension of water caused by DNAPL diffusion in the liquid phase.

During the infiltration and initial redistribution of a DNAPL in an unsaturated porous medium, its flow is so rapid that the best possible way of documenting its behavior is by obtaining photos (Figure 1 through 4). However, once static equilibrium of both water and DNAPL had been obtained, gamma-radiation attenuation was used to determine liquid saturations at 1,150 more or less evenly distributed locations. Additional gamma-radiation scans were obtained to quantify the removal of  $\text{CCl}_4$  during the vapor extraction procedures. The gamma data and analysis of the extracted vapor samples will be modeled using STOMP to compare numerical and experimental results.



**Figure 4.** Near the final DNAPL distribution, the full collapse of the capillary fringe was observable, which was attributed to a reduction of the surface tension of water caused by DNAPL diffusion in the liquid phase.

## Polymer-Ceramic Conversion of Liquid Polyaluminasilazanes for SiAlCN Ceramics

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In contrast to traditional methods for the formation of ceramic precursors, the researchers within Linan An's laboratory at the University of Central Florida synthesized liquid-phased polyaluminasilazanes by reacting a liquid polyureasilazane with aluminum isopropoxide. This unique direct chemical-to-ceramic route has recently attracted attention since it

possesses many advantages over conventional powder-based ceramic processing. For example, many unconventional structures, such as fibers (Yajima et al. 1978), coatings (Muller 1998), ceramic matrix composites (Walker et al. 1983), and ceramic-based micro-electro-mechanical systems (Liew et al. 2001) can be easily fabricated by this technique. The direct chemical-to-ceramic technique also offers a unique opportunity to manipulate compositions and structures of ceramics at atomic/nanolevels through tailoring the chemistry of the precursors; thus, new materials with chosen properties could be designed and synthesized. Amorphous SiCN and SiBCN ceramics synthesized by this technique have shown unique thermal stability (Riedel et al. 1996), creep resistance (An et al. 1998), and tunable electric properties (Ramakrishnan et al. 2001).

Professor An's recent visits to EMSL made use of the facility's 300-MHz nuclear magnetic resonance spectrometer to analyze the aluminum and silicon coordination present within the precursor and ceramic materials following progressive processing conditions. Results revealing the structural evolution of polyaluminasilazanes during pyrolysis showed that the polymer-ceramic conversion can be classified into three stages: 1) cross-linking, 2) thermal decomposition, and 3) structural rearrangement. Measurements of the thermal mechanical properties influenced by the ceramic structural alterations are in progress.

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## Correlated Topographic and Spectroscopic Imaging by Combined Atomic Force Microscopy and Optical Microscopy

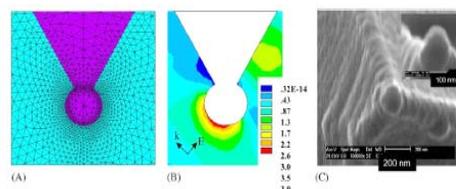
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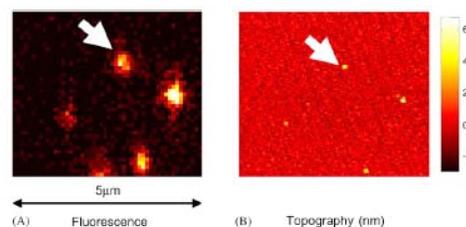
Optical microscopy has been in development for hundreds of years. Improving the contrast and resolution for biological applications has been a major endeavor. Many techniques have been tried in order to improve contrast, including fluorescence and Raman imaging. Introducing fluorescent labels to a sample allows a species to be imaged with high sensitivity and high contrast. Recently, fluorescence lifetime imaging microscopy (FLIM) was found to further improve contrast by exploiting the lifetime difference of the fluorescent species and the local environments.

Raman near-field scanning microscopy is a powerful approach to obtaining topographic and spectroscopic characterization data simultaneously for imaging biological and nanoscale systems. To achieve optical imaging at high-spatial resolution beyond the diffraction limit, aperture-less metallic scanning tips were used to enhance the laser illumination local electromagnetic field at the apex of the scanning tips. We recently published our work (Hu et al. 2004) on combined fluorescence imaging with atomic force microscope (AFM)-metallic tip enhancement, finite element method simulation of tip enhancement and their applications on AFM-tip enhanced fluorescence lifetime imaging (AFM-FLIM), and correlated AFM and FLIM imaging of living cells.

We used the frequency-domain finite element method (FEM) to characterize the near-field electromagnetic field distribution at the metallic-coated AFM tip apex by solving classical Maxwell's equations in the short-field



**Figure 5.** 3-D FEM simulation of electric field distribution in the vicinity of the coated tip structure. (A) Cross-section through the detail of finite element mesh. The geometry of the model is taken directly from the electron micrography measurements. The zoom-in mesh structure at the tip is shown in a 2-D plot. (B) Near-field distribution of the electric field in the vicinity of the Au-coated AFM tip apex. Vectors  $k$  and  $E$  represent the laser-beam propagation vector and the electric field vector, respectively. (C) Field emission scanning electron micrography of the gold-coated AFM tip. A globular gold structure at the apex of the tip is evident.

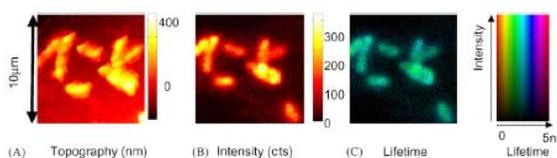


**Figure 6.** The fluorescence intensity image (A) and AFM image (B) of the same sample area containing 40-nm fluorescence nanospheres. The sample was first imaged by sample-scanning confocal fluorescence microscopy and then by tip-scanning AFM of the same area.

approximation. FEM is a well-established and reliable computational approach in electrical engineering research for simulating electromagnetic fields. An example of these simulations is shown in Figure 5. Comparison of the simulation with an image of an actual tip is shown in Figure 5C.

Using the above described tip, we performed simultaneous correlated topographic and spectroscopic imaging of fluorescent polymer nanoparticles beyond the diffraction-limited spatial resolution. Sample-scanning confocal fluorescence imaging of the sample slide was first performed to locate the fluorescent nanospheres. Then, the same sample area was imaged by tip-scanning tapping-mode AFM with gold-coated tips. Figures 6A and 6B are correlated fluorescence intensity and AFM topographic images from the same sample area. Figure 6A shows a confocal fluorescence image of a nanosphere sample on a glass coverslip. The nanospheres appear as a bright spot at a spatial resolution at about the diffraction limit ( $\sim 300$  nm).

We also explored the utility of correlated AFM/FLIM imaging on MR-1 cells expressing the MCP-YFP fusion. Since the sizes of the bacterial cells are typically at around the 1- $\mu\text{m}$  scale, which is very small for far-field optical imaging, the high-resolution imaging of AFM is important for investigating the sub-cellular structure of bacteria. The correlated AFM height image, fluorescence intensity image, and fluorescence lifetime image of a single cell are shown in Figures 7A through 7C, respectively.



**Figure 7.** Composite correlated AFM-confocal FLIM image of *S. oneidensis* bacterial cells on polylysine surface: (A) topographic image, (B) confocal fluorescence intensity, and (C) confocal fluorescence lifetime image.

Based on near-field metallic-tip enhanced microscopy and FEM simulation, we developed and applied a combined approach using AFM and optical microscopy to investigate the correlated topographic and spectroscopic information of nanoparticle and biological systems. Metallic AFM tip enhancement enabled us to obtain optical images with spatial resolution beyond the diffraction limit. Correlated topography, fluorescence intensity, and fluorescence lifetime images of living cells show high promise of biological optical imaging beyond the diffraction limit, providing information that is not obtainable using noncorrelated and far-field imaging approaches. Details on this work are published in Hu et al. 2004.

## Reference

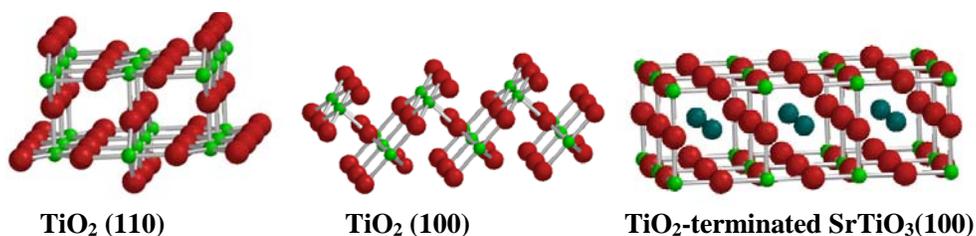
Hu D, M Micic, N Klymyshyn, YD Suh, and HP Lu. 2004. "Correlated Topographic and Spectroscopic Imaging by Combined Atomic Force Microscopy and Optical Microscopy." *Journal of Luminescence* 107(1-4):4-12.

## Adsorption and Reaction of Acetaldehyde on Stoichiometric and Defective SrTiO<sub>3</sub>(100) Surfaces

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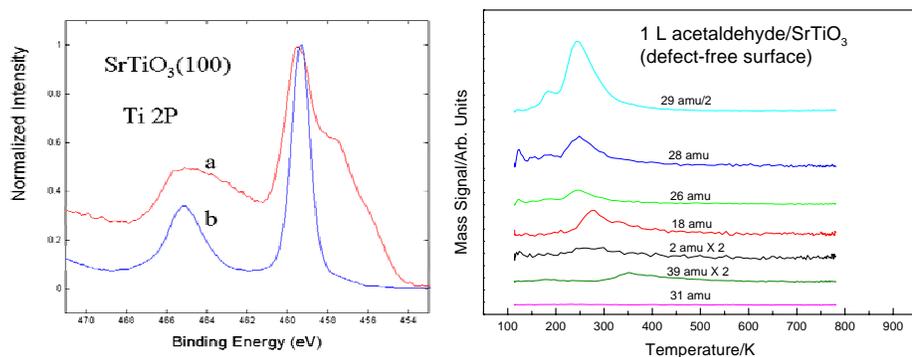
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**Figure 8.** Schematic models for the TiO<sub>2</sub>(110), TiO<sub>2</sub>(100), and TiO<sub>2</sub>-terminated SrTiO<sub>3</sub>(100), where the bigger spheres represent oxygen atoms and the smaller spheres are titanium atoms.

A fundamental understanding of the decomposition of acetaldehyde on TiO<sub>2</sub> and SrTiO<sub>3</sub> surfaces is interesting because of the complexities in the chemistry of aldehydes and the variety of coordination environments provided by these surfaces. As compared with TiO<sub>2</sub>(110) and (100) surfaces, the TiO<sub>2</sub>-terminated SrTiO<sub>3</sub>(100) surface shows unique geometric arrangements. The latter surface is rather flat with only in-plane oxygen atoms, whereas the TiO<sub>2</sub>(110) and TiO<sub>2</sub>(100) surfaces have rows of two-coordinate bridging oxygen atoms lying above the rows of titanium atoms, as observed in Figure 8.

Adsorption and reactions of acetaldehyde (CH<sub>3</sub>CHO) on stoichiometric (TiO<sub>2</sub>-terminated) and reduced SrTiO<sub>3</sub>(100) surfaces were investigated using temperature-programmed desorption (TPD) and X-ray photoelectron spectroscopy (XPS). Ar<sup>+</sup> ion bombardment was used to systematically shift the average surface oxidation state from Ti<sup>4+</sup> to Ti<sup>3+</sup>. Figure 9 displays a narrow and symmetric Ti 2p peak resulting predominantly from



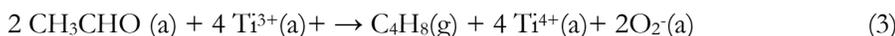
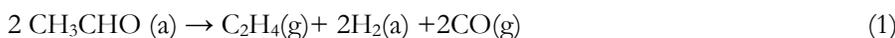
**Figure 9.** (Left) Ti 2p and O 1s XPS spectra for a sputter-reduced SrTiO<sub>3</sub>(100) surface (a) and a nearly defect-free (stoichiometric) SrTiO<sub>3</sub>(100) surface (b) at 297 K. (Right) TPD spectra monitoring 2, 15, 18, 26, 28, 29 and 31 amu, following adsorption of 1-L acetaldehyde on stoichiometric SrTiO<sub>3</sub>(100) surfaces at 110 K.

Ti<sup>4+</sup> cations on the oxidized surface, whereas the sputter-reduced surface shows a large broadening in the spin-orbit split Ti 2p peaks due to the presence of Ti<sup>3+</sup> and Ti<sup>2+</sup> cations.

Acetaldehyde adsorbs molecularly on the stoichiometric SrTiO<sub>3</sub>(100) surface that contains predominately Ti<sup>4+</sup> cations, as depicted in Figure 9. The Ti<sup>4+</sup> sites on the stoichiometric SrTiO<sub>3</sub>(100) surface are not sufficiently active for reactions such as aldol condensation, as opposed to the Ti<sup>4+</sup> ions on the TiO<sub>2</sub>(001) surface. Aldol condensation, which takes place through the reduction of an oxidized surface, occurs on both {011}- and {114}-faceted TiO<sub>2</sub>(001) surfaces containing four, five, and six coordinated cations. The enhanced reactivity of CH<sub>3</sub>CHO on the TiO<sub>2</sub>(001) surfaces can be attributed to the unique structures of these surfaces that possess a variety of surface sites.

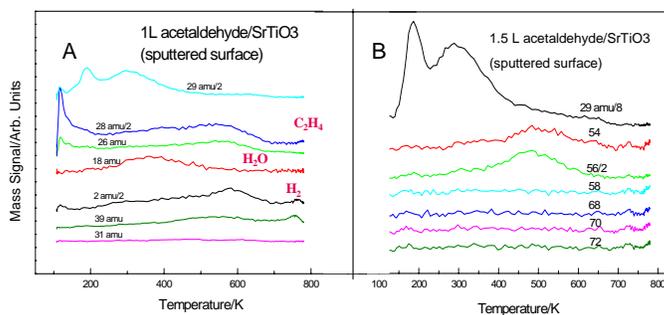
Decomposition and redox reactions of acetaldehyde occur in the presence of surface defects created by Ar<sup>+</sup> sputtering, as indicated by the TPD results shown in Figure 10. The decomposition products include H<sub>2</sub> (m/e = 2 amu), C<sub>2</sub>H<sub>4</sub> (m/e = 28, 27, 26 amu), CO (m/e = 28), C<sub>4</sub>H<sub>6</sub> (m/e = 54 amu), and C<sub>4</sub>H<sub>8</sub> (m/e = 56 amu). The TPD results clearly indicate that reductive coupling, to produce C<sub>2</sub>H<sub>4</sub> and C<sub>4</sub>H<sub>8</sub>, is the main reaction pathway for decomposition of acetaldehyde on the sputter-reduced SrTiO<sub>3</sub>(100) surface.

Equations 1 and 2 illustrate these pathways (here “g” and “a” stand for “gas” and “adsorbate,” respectively, and Ti<sup>3+</sup> used here represents reduced cations created by Ar<sup>+</sup> sputtering). Further dehydrogenation of C<sub>4</sub>H<sub>8</sub> and formation of butadiene (C<sub>4</sub>H<sub>6</sub>, m/e 54) are also observed during TPD.



Equation 3 shows that the bimolecular coupling to produce C<sub>4</sub>H<sub>8</sub> may also involve the oxidation of Ti<sup>3+</sup> to Ti<sup>4+</sup>. The sputter-induced damage is found to be completely healed by annealing during the TPD process, indicating that dissociation of acetaldehyde most likely oxidizes the reduced surface. Similar reductive coupling also takes place on the reduced TiO<sub>2</sub>(001) following

adsorption of acetaldehyde on these surfaces, suggesting that reduced titanium cation sites are responsible for the initiation of the coupling reactions. The differences in reactivity between stoichiometric SrTiO<sub>3</sub> and TiO<sub>2</sub> surfaces presumably originate from the unique geometric and electronic structure of the SrTiO<sub>3</sub>(100) surfaces.



**Figure 10.** TPD spectra monitoring 29, 54, 58, 68, 70 and 72 amu following adsorption of 1.5-L acetaldehyde (B) on the sputtering-reduced SrTiO<sub>3</sub>(100) surfaces at 120 K.

## Multidimensional Mass Spectrometric Analysis of Breast Cancer Membrane Proteomes

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Proteins associated with plasma cell membranes participate in multiple cell-environment interactions including cell-cell communications, cell-extracellular interactions, locomotion and migration, and cell signaling. Membrane-associated proteins account for 70% of all known pharmaceutical drug targets, and are also targets for a number of new drug and antibody-based therapeutics in cancer. We undertook a study to define the membrane proteome of breast cancers. In order to capture the maximum number of breast cancer-associated proteins, we analyzed the membrane proteome of a panel of breast cancer cell lines using a combination of subcellular fractionation, separation by strong cation exchange chromatography, and reversed-phase capillary liquid chromatography followed by tandem mass spectrometry. The proteins identified were investigated further in an effort to identify plasma membrane-associated proteins (PMAPs) and groups of proteins over-represented in the breast cell-line panel. Additional information derived from gene expression datasets were used to identify proteins that may have a potential relevance to breast cancer.

Four breast cancer cell lines [SKBR-3, MDA-MB-231, BT-474, and an MCF7-c18 transfectant cell line over-expressing the ERBB2 receptor tyrosine kinase (RTK)] were cultured and used to make up the breast cancer panel. Membrane-enriched fractions were prepared separately for all four cell lines and then pooled into a single mixture. All sample aliquots combined to produce 202 fractions, which produced 724,566 mass spectrometry/mass spectrometry spectra. This corresponded to a total of 42,250 high-scoring peptides matching 2,344 proteins listed in the September 2003 freeze of the human International Protein Index database (<http://www.ebi.ac.uk/IPI/IPIhelp.html>). Among all proteins identified, 28% had less than 10% sequence coverage, 65% had 20% to 50% sequence coverage, and 6% had sequence coverages of greater than 60%.

Querying of the UniGene database revealed more than 1,905 unique genes represented by this set of proteins. 1,525 (80%) of these unique genes (identified from all three aliquots) were mapped to the gene ontology (GO) database and classified according to molecular function and cellular component categories. The combination of both molecular function and cellular component categories yielded 312 proteins that were associated with the plasma membrane, as evidenced by both functional and localization information. Since GO categories are often incomplete and ambiguous, several proteins were manually inspected for association with the plasma membrane. Manual inspection revealed an additional 40 PMAPs. Most proteins in the subset of 352 PMAPs were associated with signal transducer activity, binding, and transporter activities. The sub-categorization of our dataset according to the GO database resulted in many proteins putatively involved in immune response, apoptosis, catalytic activity and several other cellular processes. According to the protein families (PFAM) database, 20 protein sequence domain/families were well represented (greater than five member proteins) in our collection of PMAPs. Many of these domains include well-

conserved transmembrane-bound domains and several groups of proteins known to be membrane-associated. Among those identified were the immunoglobulin domain (~100 residues); the fibronectin type III domain (~100 residues); the EGF-like domain (30-40 residues); the SH3 domains (~50 residues); the WD domain; G-beta repeat (~40 residues); the FERM (~150 residues) domain; the PDZ domains (80 to 90 residues); the tubulin domains; the sterile alpha motif (>70 residues); the cadherin domain; and the low-density lipoprotein receptor domain. Well-represented protein families included members of the ADP-ribosylation factor family, the ABC transporters, the Ras family of GTPases, the GGL (Guanine nucleotide binding G-protein) family, and the Tetraspanin family.

Using the procedure described by Hosack et al., protein groupings based on functional domains in several protein signature databases were used to examine whether any populations of proteins were abundant in our sample. Two protein categories (as defined in the PFAM and Simple Modular Architecture Research Tool (SMART) databases) contained a significantly (less than 0.01) higher number of proteins in our sample than would be expected by random chance. Four proteins belonging to the SNF-7 homologues (PFAM, PF03357) domain were identified in our sample. This family of proteins is involved in formation of multivesicular bodies, which play a critical role in the recycling and degradation of membrane proteins (i.e., activated cell surface receptors). Thirteen proteins belonging to the PDZ/DHR/GLGF (SMART, SM00228) domain were also identified. Members of this group of proteins are thought to direct the targeting of signaling molecules to sub-membranous sites. The PDZ/DHR/GLGF domain group included proteins frequently associated with the plasma membrane, a compartment where high concentrations of phosphatidylinositol 4,5-bisphosphate are found. They interact directly with several ephrin-related RTKs, the ERBB2 RTK, and with C-terminal sequences derived from other transmembrane receptors.

In summary, our study identified a large collection of plasma membrane-associated proteins from a breast cancer cell-line panel using high-throughput tandem mass spectrometry techniques. Several tools allowed us to create a membrane proteome profile of this set of cell lines. In addition, we were able to combine gene expression data with proteomic data to identify several PMAPs that may play important roles in the initiation and progression of breast carcinomas. Since we analyzed a limited number of specimens, additional experiments using high-throughput techniques, such as mRNA in-situ hybridization or immunohistochemical analysis on tissue-microarrays, are required to determine how commonly these genes are differentially expressed. Additional analysis of these genes and the biochemical pathways in which they are involved will not only further our understanding of breast oncogenesis, but will also provide new and valuable targets for translational research.

## Reference

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## Geometry Optimizations of Aqueous Aluminum Clusters

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We conducted first-principle calculations of the surface morphology of the {100} face growth hillock of the mineral Archerite ( $[\text{K},\text{NH}_4]\text{H}_2\text{PO}_4$ ), which is used extensively in industrial applications—for example, at the National Ignition Facility at Lawrence Livermore National Laboratory. To perform the calculations, we used the plane-wave pseudopotential density-functional theory (PWPS-DFT) and Car-Parrinello *ab initio* molecular dynamics functions of the NWChem software package. The PWPS-DFT function provides a good economy of calculation time, especially for systems as large as this one, yet retains accurate energy prediction. Calculations for surfaces and bulk phases were found to be periodic, and those for growth units were aperiodic. Step energies were also calculated using the difference between a step and a slab, with the same number of atoms and same cell dimensions. The {100} surface energy was calculated by subtracting the total PSPW energy of a bulk phase from the energy of the same cell, but with space added in the {100} direction, so that the area of the calculation and the number of atoms were the same. Attachment energies were calculated by subtracting the energy of a step and the energy of the isolated growth unit from the energy of the step with growth unit adsorbed. Typical simulations were run for ~2000 iterations at 5 a.u. per time step ( $1.2 \times 10^{-16}$  seconds per time step) with a steady state reached after ~1000 iterations.

We found qualitative consistency between the calculations and experiment. Attachment energies to the {010} facing step were -4.6 and -4.7 eV. The corresponding calculation for the slow {001} direction was -5.7 eV, which is much more favorable than attachment to either the fast direction or the first monomers on the slow direction. Therefore, it is likely that in the slow {001} direction, the initial adsorption of new material to the step is limiting the rate and, that once it has been adsorbed, the second unit adsorbs very quickly and reproduces the step.

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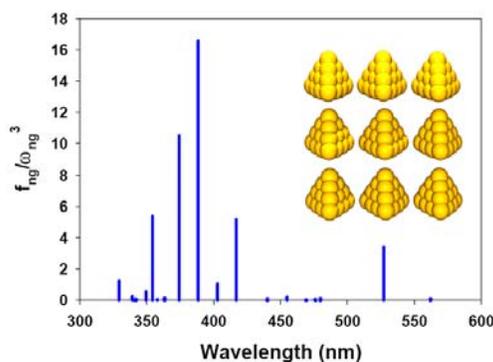
## Remarkable Second-Order Optical Nonlinearity of Nano-Sized Au<sub>20</sub> Cluster: A TDDFT Study

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The recently discovered Au<sub>20</sub> nanocluster is a very stable tetrahedral molecule that has great potential in catalysis, optical, and non-linear optical applications (Li et al. 2003). In the present work, the dipole polarizability, static first hyperpolarizability, and UV-Vis spectrum of Au<sub>20</sub> have been investigated by using time-dependent density functional response theory (TDDFT). It was found that the Au<sub>20</sub> cluster possesses remarkably large molecular second-order optical nonlinearity with the first hyperpolarizability ( $\beta_{xyz}$ ) calculated to be  $14.3 \times 10^{-30}$  esu, which is about 150 times larger than the average hyperpolarizability of the organic urea molecule. The analysis of the low-energy absorption band suggests that the charge transfer from the edged gold atoms to the vertex atoms plays the key role in nonlinear optical response of Au<sub>20</sub> (Figure 11) (Wu et al. 2004). Since Au<sub>20</sub> cluster is a fragment of the fcc lattice of bulk gold, it is very promising to apply this nanocluster in molecular opto-electronic devices and monolayer film materials.



**Figure 11.** The seven major transitions responsible for the non-linear optic response of Au<sub>20</sub> nanocluster (the inset shows an array of 9 Au<sub>20</sub> molecules).

This research was performed in part using EMSL's Molecular Science Computing Facility.

### References

Li J, X Li, HJ Zhai, and LS Wang. 2003. "Au<sub>20</sub>: A Tetrahedral Cluster." *Science* 299(5608):864-867.

Wu K, J Li, and C Lin. 2004. "Remarkable Second-Order Optical Nonlinearity of Nano-Sized Au<sub>20</sub> Cluster: A TDDFT Study." *Chemical Physics Letters* 388(4-6):353-357.

## Significant Interactions Between Uranium and Noble-Gas Atoms: Coordination of the $\text{UO}_2^+$ Cation by Ne, Ar, Kr, and Xe Atoms

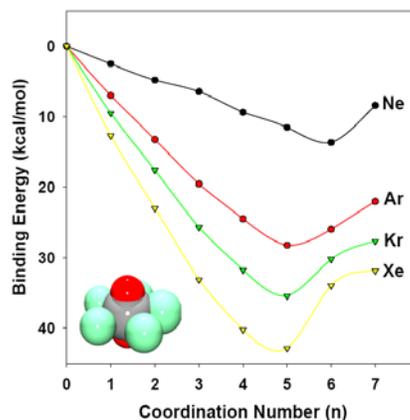
Wang X,<sup>(a)</sup> L Andrews,<sup>(a)</sup> J Li,<sup>(b)</sup> and BE Bursten<sup>(c)</sup>

(a) University of Virginia, Charlottesville, Virginia

(b) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

(c) The Ohio State University, Columbus, Ohio

Following the previous discovery of direct bonding interactions between uranium atoms and noble-gas (Ng) atoms in the matrix-isolated neutral CUO and  $\text{UO}_2$  molecules (Li et al. 2002; Li et al. 2004), U(V) in  $\text{UO}_2^+$  monocation is found to form a variety of noble-gas complexes from the reaction of laser-ablated uranium atoms with  $\text{O}_2$  and subsequent isolation in solid noble-gas matrices (Wang et al. 2004). Relativistic density functional and *ab initio* coupled cluster CCSD(T) calculations indicate that the uranium-Ng bonding in these complexes is stronger than the uranium-Ng bonds that involve neutral CUO and  $\text{UO}_2$ , largely because of the combination of electron-donation and ion-induced dipole interactions. Theoretical calculations of the optimal coordination number of  $\text{UO}_2^+$  ion by Ng atoms predict the formation of  $\text{UO}_2(\text{Ne})^{6+}$ ,  $\text{UO}_2(\text{Ar})^{5+}$ ,  $\text{UO}_2(\text{Kr})^{5+}$ ,  $\text{UO}_2(\text{Xe})^{5+}$  complexes in the noble-gas matrices (Figure 12). Matrix-isolated new species of  $\text{UO}_2(\text{Ng})_m(\text{Ng}')_n^+$  are also identified from the experimentally measured infrared spectra. This research was performed in part using EMSL's Molecular Science Computing Facility.



**Figure 12.** The calculated binding energy curves for  $\text{UO}_2(\text{Ng})_n^+$  (Ng = Ne, Ar, Kr, Xe). The inset shows the structure of the  $\text{UO}_2(\text{Ar})^{5+}$  molecule.

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- Wang X, L Andrews, J Li, and BE Bursten. 2004. "Significant Interactions Between Uranium and Noble-Gas Atoms: Coordination of the  $\text{UO}_2^+$  Cation by Ne, Ar, Kr, and Xe Atoms." *Angewandte Chemie International Edition* 43(19):2554-2557.

## Noble Gas–Uranium Coordination and Intersystem Crossing for the $\text{CUO}(\text{Ne})_x(\text{Ng})_n$ ( $\text{Ng} = \text{Ar}, \text{Kr}, \text{Xe}$ ) Complexes in Solid Neon

L Andrews,<sup>(a)</sup> B Liang,<sup>(a)</sup> J Li,<sup>(b)</sup> and BE Bursten<sup>(c)</sup>

(a) University of Virginia, Charlottesville, Virginia

(b) W.R. Wiley Environmental Molecular Sciences Laboratory, Richland, Washington

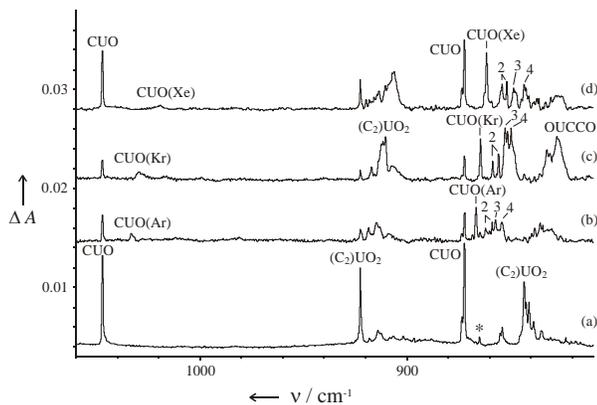
(c) The Ohio State University, Columbus, Ohio

Atomic uranium excited by laser ablation reacts with CO in excess neon to produce the novel CUO molecule, which forms weak complexes  $\text{CUO}(\text{Ne})_m$  with neon and stronger complexes  $\text{CUO}(\text{Ne})_x(\text{Ng})_n$  ( $\text{Ng} = \text{Ar}, \text{Kr}, \text{Xe}$ ) when the heavier noble gas atoms are present. Heavier  $\text{CUO}(\text{Ne})_{m-1}(\text{Ng})$  complexes are identified through the effects of CO isotopic and noble gas (Ng) substitution on the neon matrix infrared spectra and by comparison to density functional theory (DFT) frequency calculations on the model complexes  $\text{CUO}(\text{Ng})$  ( $\text{Ng} = \text{Ne}, \text{Ar}, \text{Kr}, \text{Xe}$ ). The U–C and U–O stretching frequencies of the  $\text{CUO}(\text{Ne})_{m-1}(\text{Ng})$  complexes are slightly red shifted from the 1047 and 872  $\text{cm}^{-1}$  frequencies for the  $^1\Sigma^+$

CUO ground state neon complex, which identifies singlet ground state  $\text{CUO}(\text{Ne})_{m-1}(\text{Ng})$  complexes in solid neon (Figure 13) (Andrews et al. 2004). The next singlet  $\text{CUO}(\text{Ne})_x(\text{Ng})_2$  complexes in excess neon follow in like manner. However, stretching modes and the isotopic shifts of the higher  $\text{CUO}(\text{Ne})_x(\text{Ng})_n$  ( $n > 2$ ) complexes approach those of the pure argon matrix  $\text{CUO}(\text{Ar})_n$  complex, which characterizes triplet ground state complexes by comparison to DFT frequency calculations. These experimental and calculations results indicate that the ground state reversal of CUO is a consequence of multiple coordination of CUO by heavy Ng atoms.

### Reference

Andrews L, B Liang, J Li, and BE Bursten. 2004. "Noble Gas-Uranium Coordination and Intersystem Crossing for the  $\text{CUO}(\text{Ne})_x(\text{Ng})_n$  ( $\text{Ng} = \text{Ar}, \text{Kr}, \text{Xe}$ ) Complexes in Solid Neon." *New Journal of Chemistry* 28(2):289-294.



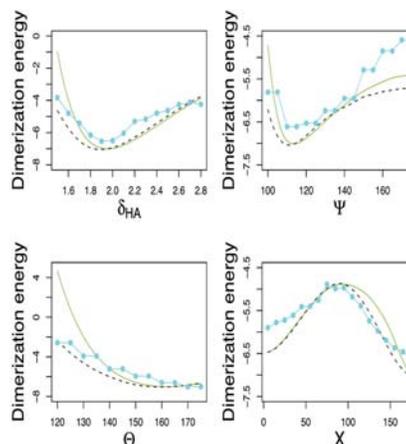
**Figure 13.** Infrared spectra in the 1060–810  $\text{cm}^{-1}$  region for laser-ablated U atom, 0.1% CO, Ng reaction products in excess neon at 3.5 K after sample deposition, photolysis and annealing to 12–13 K: (a) pure neon, (b) 1% Ar in neon, (c) 0.5% Kr in neon, and (d) 0.3% Xe in neon.

## Close Agreement Between the Orientation Dependence of Hydrogen Bonds Observed in Protein Structures and Quantum Mechanical Calculations

AV Morozov,<sup>(a)</sup> T Kortemme,<sup>(a)</sup> KL Tsemekhman,<sup>(a)</sup> and D Baker<sup>(a)</sup>

(a) University of Washington, Seattle, Washington

Hydrogen bonding is weakly covalent and mostly an electrostatic interaction between a weakly acidic donor group and an acceptor atom that bears a lone pair of electrons. These chemical interactions play a central role in determining the structure and function of proteins; therefore, an accurate description is essential for a proper description of protein interactions. With energies of 12 to 30 kJ/mol, hydrogen bonds present a significant computational challenge to accurately describe. In this work (Morozov et al. 2004), the orientation and distance dependence of hydrogen bonds are investigated by both structural analysis of the Protein Data Bank and electronic structure calculations with NWChem. The latter were performed using an aug-cc-pVDZ basis set with both density functional theory and MP2 levels of theory. The model system used in the quantum-mechanical calculations was taken to be a formamide dimer (Figure 14). The calculations reveal a close correspondence between the quantum-mechanical energy landscape and that inferred from the distribution of side-chain-side-chain hydrogen bonds in protein structures from the Protein Data Bank archive. The same comparison performed for molecular mechanics force fields shows systematic deviations from both experimental and electronic structure results. These results suggest that a purely electrostatic approach to the description of hydrogen bonding in standard molecular mechanics force fields is of limited accuracy. To attain a better description of hydrogen bonding may require a next generation of molecular force fields that incorporate polarizabilities, higher-order multipole interactions, etc.



**Figure 14.** Formamide dimer hydrogen bonding energies (kcal/mol) vs.  $\delta_{\text{HA}}$  (Å),  $\Psi$ ,  $\theta$ , and  $X$ (°).

### Reference

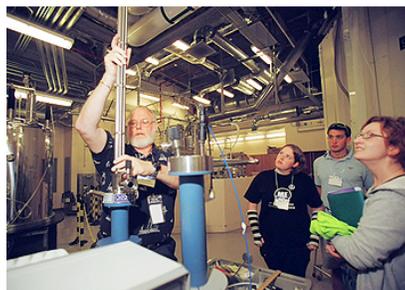
Morozov AV, T Kortemme, K Tsemekhman, and D Baker. 2004. "Close Agreement Between the Orientation Dependence of Hydrogen Bonds Observed in Protein Structures and Quantum Mechanical Calculations." *Proceedings of the National Academy of Sciences of the United States of America* 101(18):6946-6951.

## Awards and Recognition

**EMSL User Featured in *Science*.** Lai-Sheng Wang, Washington State University, Richland, Washington, was featured in the May 28 edition of *Science* in a special section, "Many Origins, One Destination," that highlights the stories of six foreign-born scientists and their interest in coming to study and work in the United States, and their impact on U.S. academic science. This is a very compelling feature and a subject of great relevance in the scientific community.

## Professional/Community Service

**EMSL2004 Users Meeting.** On June 14 – 16, 2004, the High-Field Magnetic Resonance Facility hosted the EMSL2004 technical meeting, "Bridging Technologies in Structural Biology." More than 60 participants from academia, industry, and other national laboratories attended. The first day focused on how a wide variety of techniques, including X-ray crystallography, cryo-electron microscopy, small-angle neutron scattering, and electron paramagnetic spectroscopy, along with NMR would be needed to tackle future grand challenges in biology and structural genomics. The second and third days focused on user research performed at EMSL in the High-Field Magnetic Resonance Facility. During the three-day meeting attendees took part in poster sessions and tours of EMSL and had the opportunity to exchange ideas with the EMSL User Advisory Committee. Invited speakers included the following:



**Figure 15.** EMSL2004 participants in the EMSL Nuclear Magnetic Resonance Facility with PNNL researcher Paul Ellis, left.

- Michael Chapman, Florida State University, "Holistic Macromolecular Models—When One Technique is Not Enough"
- Thomas Szyperski, University of Buffalo, "NMR Methods Enabling Rapid Data Collection"
- Jinkui Zhao, Oak Ridge National Laboratory, "Small-Angle Neutron Scattering in Structural Biology"
- Stanley Opella, University of California, San Diego, "NMR Structure Determination of Mercury Transport Membrane Proteins"
- James Penner-Hahn, University of Michigan, "Characterization of 'Spectroscopically Challenged' Metals: Zinc in Biological Systems—X-ray Spectroscopy"

- Rachel Kleivit, University of Washington, “Assembly of Multi-Component Protein Complexes: NMR Studies of a BRCA1-BARD1 Ubiquitin Ligase Complex”
- Huilin Li, Brookhaven National Laboratory, “The Expanding Role of Cryo-Electron Microscopy in Structural and Cell Biology”
- Colin Fyfe, University of British Columbia, “High-Field Solid-State NMR Studies of Inorganic Materials at the Pacific Northwest National Laboratory”
- Thomas DiChristina, Georgia Institute of Technology, “New Insights into the Molecular Mechanism of Microbial Metal Respiration.”

#### **EMSL Hosts Surface Analysis 2004/Pacific Northwest**

#### **American Vacuum Society 2004 Meeting.**

On June 15 – 18, 2004, EMSL hosted more than 150 participants at the joint Surface Analysis 2004-Pacific Northwest American Vacuum Society meeting, organized by the Interfacial and Nanoscale Science Facility and PNNL staff. Several speakers (see Figure 16) participated this year, including Colin Fyfe, University of British Columbia; Paul Cremer, Texas A&M University; and Marc Porter, Iowa State University. During this meeting, papers were given in biomaterials and interfaces, nanoscience, catalysis, oxide thin films, and advanced methods, and more than 50 posters were presented—including several local and northwest winners of the high school, undergraduate, and graduate student poster competition. Of the eight poster competition winners, three are based at EMSL and two are users working with EMSL staff.



**Figure 16.** As one of the speakers at this year's Surface Analysis 2004/Pacific Northwest American Vacuum Society 2004 Meeting, Claude Henry, CMC2-CNRS, Marseille, France, presents his work in the talk "Nucleation, Growth and Reactivity of Gold Particles on MgO(100)."

**Clay Minerals Society 41<sup>st</sup> Annual Meeting.** EMSL researcher Paul Gassman and user Jim Amonette chaired the 2004 Clay Minerals Society 41<sup>st</sup> Annual Meeting on June 19-24, 2004, in Richland Washington. The meeting was a great success, with 185 attendees, 74 of whom registered for the Methods for Investigating Microbial-Mineral Interactions workshop in the EMSL auditorium, and 51 of whom participated in EMSL laboratory tours. A total of 113 papers were presented (86 orally), covering a wide range of fundamental, practical topics, and the latest advancements in the uses of clay minerals.

**Environmental Spectroscopy Symposium.** Nancy Foster-Mills, Environmental Spectroscopy and Biogeochemistry Facility Technical Group Leader, organized a symposium on environmental spectroscopy that focused on presentations related to the application of various optical spectroscopies in environmental research. The symposium was held at the

Joint Regional Meeting of the Northwest and Rocky Mountain Sections of the American Chemical Society on June 6-9, 2004, at Utah State University in Logan Utah.

**Instrument Development Laboratory, Washington State University Promote Education and Science.** Members of EMSL's Instrument Development Laboratory (IDL) and the Institute of Electrical and Electronics Engineers (IEEE) student chapter at Washington State University (WSU) are teaming with eastern Washington high schools and Washington's Mathematics Engineering Science Achievement program to promote science and engineering education through robotics. The result of this outreach has not only resulted in successful educational promotion, but it has also strengthened university, laboratory, and public school communications.

In the past, PNNL and Southridge High School in Kennewick, Washington—under the coordination of IDL Technical Group Leader Gordon Anderson and Southridge Engineering Technology instructor Jim Hendricks—have held SUMO robotics competitions with the goal of students building a completely autonomous robot that pushes its opponent out of a small circular ring. IDL staff member Gabriel Guillen created a simple circuit for students to use as a base platform for robot construction. The students are given a small circuit board and electronic parts and must learn how to read circuit schematics and parts list, identify parts and their function, as well as design a robot chassis to meet competition specifications. Students also learn how to modify servo and direct current motors to mobilize their robot, and how to program the robot in a simple programming language.

Recently, IDL staff member Brian La Marche, along with the IEEE chapter and WSU's Electrical Engineering and Computer Science (EECS) Department, extended robotics educational outreach to the Pullman, Washington, area. Working remotely with Hendricks, Anderson, and Jim Alzheimer of Battelle Robotic Automation Technology Society, they created the WSU IEEE SUMO Robotics club consisting of electrical engineering, computer science, computer engineering, and mechanical engineering students who volunteer their time to teach robot construction at eastern Washington high schools. For example, Pullman's physics classes learned the engineering and science skills of building robots using Guillen's circuit board. The IEEE SUMO Robotics club has also visited Spokane area schools. This outreach culminated in the IEEE chapter's first SUMO robotics competition at the end of WSU's spring semester. The competition was held in conjunction with the EECS Department Open House to allow Southridge, Pullman, Lewis and Clark, and Shadle high school students to attend a poster session of the EECS senior design projects.

IDL staff members Eric Choi and Thomas Seim also attended the competition and EECS Open House, where they were invited to attend the Executive Advisory Board for the EECS Department by EECS Alumni and Corporate Relations Director Kathleen Warren.

**Energy Smart Data Center.** On June 22, 2004, PNNL hosted a kickoff meeting of the Energy Smart Data Center collaboration project with Isothermal Systems Research (ISR). This project will support research of exotic cooling methods for commodity hardware. Representatives from PNNL, ISR, Tessra, Opus Innovations, and Intel were present at the meeting.

**Advanced Storage Technologies.** PNNL announced a research alliance aimed at enabling a new generation of fast and efficient storage technologies for data-intensive computing. Part of a long-term collaboration between PNNL and Silicon Graphics (SGI), the alliance will involve researching options for more than 2.5 petabytes of storage during the next two years. The effort combines the expertise of SGI and PNNL in advanced storage technologies to address national priorities of the Laboratory in the chemical, physical, and biological sciences. SGI will deliver a single 380-terabyte file system to EMSL this summer as part of the alliance's first phase. See <http://www.pnl.gov/main/highlights/sgi.html> for more information.

**Elisabeth and Robert Moore Observatory.** Beginning early this spring, IDL staff member Ken Swanson became involved with overseeing the specification and design of the Elisabeth and Robert Moore Observatory that is currently in construction on the campus of Columbia Basin College (CBC) in Pasco, Washington. Swanson organized and led committee meetings and provided his astronomical expertise with the Rattlesnake Mountain Observatory to assist with technical needs. Construction of the observatory commenced with a ground-breaking ceremony on June 21. The 1,000-square-foot facility is scheduled for completion this fall and will house a 16-inch Meade Schmidt-Cassegrain reflecting telescope and Ash Dome. The facility is a result of a \$1.1-million donation by Bob Moore in support of CBC's Washington Institute for Science Education program. Several PNNL staff members and community members are also involved with this effort.

**MSCF Computational Grand Challenges.** The call for Computational Grand Challenge application proposals was successfully completed and is now closed. From the initial 17 letters of intent, 11 full proposals were submitted for review with several others submitting smaller pilot projects instead. An internal review was completed of the 11 proposals, and the proposals are now being sent for external scientific review. The projects were categorized into one of four EMSL mission areas based on the judgment of the internal reviewers. Table 1 shows these four areas of research and a summary of the requested computing hours for each.

Areas of Research	Numbers Submitted	Requested Computing Hours/Year
Chemistry	6	4,070,000
Biology	4	3,392,000
Environmental Science/Subsurface	1	500,000
Climate	0	0
<b>Total</b>	<b>11</b>	<b>7,962,000</b>

**Table 1. Requested computing time for EMSL Computational Grand Challenges.**

## Major Facility Upgrades

**NWChem.** The worldwide NWChem user community requested capabilities for studies of reactive systems and, in some cases, collaborated in the development and enhancement of many of the new NWChem functions, including coupled-cluster methods, density functional theory, and Q-HOP. These new functions enable researchers to address scientific questions that are relevant not only to DOE mission areas, but also to everyday chemical processes. One hundred scientists downloaded Version 4.6 of NWChem within the first week of its release. The number of user agreements worldwide is now nearly a thousand.

More information about the NWChem Version 4.6 release is available at <http://www.emsl.pnl.gov/docs/nwchem/nwchem.html>.

**Ecce.** The new Ecce Version 3.2 provides users with enhanced features supporting molecular dynamics calculations, including a force field editor and topology viewer. A new tool—the DNA toolkit—has also been added to Ecce’s arsenal. The DNA toolkit creates model segments of double-stranded DNA from arbitrary combinations of the four base pairs that are fundamental to all life. The new repertoire of capabilities in Ecce has increased the accessibility of powerful modeling tools that can be employed to understand critical processes, such as DNA-protein interactions and catalytic reactions. With nearly five new user agreements each week, Ecce has been distributed to more than 500 sites worldwide, from Europe to South America to Asia.

More information about the Ecce Version 3.2 release is available at <http://ecce.emsl.pnl.gov>.

## News Coverage

On June 22, 2004, ITworld.com article "[Apple Adds HPC Customer but Falls from Top500](#)" quoted Scott Studham, manager of computer operations with the Pacific Northwest National Laboratory's Molecular Science Computing Facility.

On June 22, 2004, PR Newswire posted the article "[PNNL, SGI to Team on Storage Technology Development for Data-Intensive Computing](#)".

On June 23, 2004, businesswire.com posted "[Breakthrough HP Technology Yields up to 100 Times More Bandwidth for Linux Clusters](#)".

On June 23, 2004, eetimes.com posted "[HP Eases I/O Bandwidth on Grids](#)".

On June 24, 2004, Internetnews.com posted the article "[PNNL, SGI Think Big](#)". The article discusses the PNNL/Silicon Graphics partnership to develop new storage technologies for data-intensive computing.

On June 25, 2004, Computerweekly.com posted the article "[HP Offers 100 Times More Linux Cluster Bandwidth](#)".

On June 26, 2004, linuxelectronics.com posted "[Lustre File System to Provide Foundation of High Performance Computing at PNNL](#)". This article discusses how PNNL will conduct research into "active storage," a groundbreaking effort to shift computation and transformation of data from client computers to storage devices.

## Visiting Users

### Chemistry and Physics of Complex Systems Facility

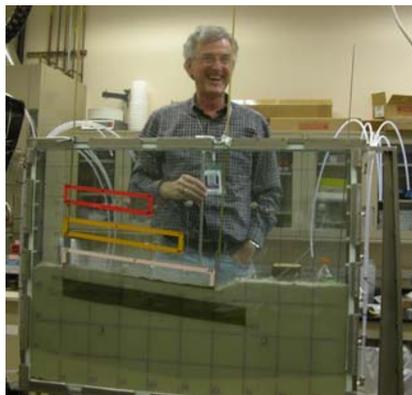
- Jormarie Alvarez, Purdue University, West Lafayette, Indiana, participated in the Interfacial and Condensed Phase Chemical Physics Summer Research Institute and worked on the study "Dissociative Charge Inversion of Peptides by Surface-Induced Dissociation."
- Benjamin Arthurs, Washington State University, Pullman, Washington, worked on the study "Image Acquisition and Analysis of Fluorescent Biological Samples."
- Emily Ashjian, Young Women in Science Program, Southridge High School, Kennewick, Washington, Brian Estes, Gonzaga University, Spokane, Washington, and Brooke Holben, Washington State University, Pullman, Washington worked on the study "Electron-Induced Genomic Instability."

- Olexandr Bondarchuk, University of Texas, Austin, Texas, worked on the study “Atomically Resolved Studies of Transition Metal Oxides.”
- Jason Han, Washington State University, Pullman, Washington, participated in the Interfacial and Condensed Phase Chemical Physics Summer Research Institute and worked on the study “Single Molecule Dynamics of Protein DNA Interactions.”
- Jenny Hand, Colorado State University, Fort Collins, Colorado, worked on the “Single Particle Analysis of Smoke Aerosols During the Summer 2002 Yosemite Aerosol Characterization Study.”
- Janine Herring, Georgia Institute of Technology, Atlanta, Georgia, worked on the study “Photon-Stimulated Desorption of Cations from Ionic Solutions.”
- Alexandre Kavetski, Khlopin Radium Institute, St. Petersburg, Russia, worked on the study “Electron Stimulated Reactions in Thin Water Films.”
- David Laman, Central Washington University, Ellensburg, Washington, participated in the Interfacial and Condensed Phase Chemical Physics Summer Research Institute and worked on the study “Charge Separation Kinetics in the  $\alpha$ -Cr<sub>2</sub>O<sub>3</sub>/ $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> System.”
- Yigal Lilach, University of California, Santa Barbara, Goleta, California, gave the seminar “Photochemistry of Oriented and Caged Adsorbates.”
- Alan Maccarone, University of Colorado, Boulder, Colorado, worked on the study “Second Harmonic Generation from Organic Water/Air Interfaces.”
- Arthur Maki, retired professor from Oregon State University, Mill Creek, Washington, worked on the study “High Resolution Infrared Spectroscopy of Boron Trifluoride.”
- Richard Osgood, Jr., Columbia University, New York, New York, visited EMSL to discuss collaborative research opportunities.
- David Panther, George Fox University, Newburg, Oregon, worked on the study “Single Molecule Approach for Understanding EGFR Molecular Interactions.”
- Luis Rodriguez, National Cancer Institute, Bethesda, Maryland, worked on the study “Development of Multi-Functional Microscopy (MFM) for Cancer and AIDS Research.”
- Philipp Schumann, Johannes Gutenberg-Universitat, Mainz, Germany, worked on the ongoing research collaboration “High-Resolution Atomic Spectroscopy as Basis for Development of Analytical Methods.”
- Steven Tait, University of Washington, Seattle, Washington, participated in the Interfacial and Condensed Phase Chemical Physics Summer Research Institute and worked on the study “Pd Nanoclusters Supported on MgO(100): Effects of Cluster Size on Chemisorption Properties.”

- Hai Wang, University of Delaware, Newark, Delaware, gave the seminar “Synthesis and Characterization of Ultrafine, Ultra-Uniform and Phase-Pure TiO<sub>2</sub> Nanoparticles.”
- Zhiwei Yang, University of Delaware, Newark, Delaware, participated in the Interfacial and Condensed Phase Chemical Physics Summer Research Institute and worked on the study “Chemical Characterization of Heterogeneous Inclusions in Soot Particles.”

## Environmental Spectroscopy and Biogeochemistry Facility

- Christopher Cahill, George Washington University, Washington, D.C., gave a seminar on novel uranyl and lanthanide compounds. He also met with PNNL scientists Eugene Ilton, Nancy Hess, and Zheming Wang to discuss becoming an EMSL user and future collaborations that would employ spectroscopic methods (Raman and time-resolved laser-induced fluorescence system) to help characterize synthetic uranyl and lanthanide framework compounds.
- Jacob Dane (Figure 17), Auburn University, Auburn, Alabama, in collaboration with PNNL researcher Mart Oostrom and EMSL scientist Tom Wietsma, conducted a detailed flow cell experiment to investigate the flow and transport behavior of a DNAPL containing carbon tetrachloride in heterogeneous Hanford Site porous materials. The DNAPL composition reflects the nonaqueous phase mixture disposed of at the Hanford Site in the 1950s and 1960s. The behavior of different DNAPL forms (entrapped, residual, and free) will be investigated in a fluctuating water table scenario. The experiment contains a remediation component where the soil vapor extraction technique is used to remove carbon tetrachloride from the unsaturated zone.
- Baohua Gu, Oak Ridge National Laboratory, Oak Ridge, Tennessee, and Zheming Wang and Chongxuan Liu, Pacific Northwest National Laboratory, Richland, Washington, collaborated on the investigation of U(VI) speciation and its influence on microbial reduction in presence of humic substances. Cryogenic fluorescence spectra of a series of uranyl solutions in the presence and absence of humic acid, along with other metal ions, such as Ca(II) and Ni(II), as well as carbonate in culture media have been acquired. Preliminary analysis of the results suggested that while the presence of both humic acid and transition metal ions influences the speciation of U(VI), the complexation of bicarbonate with uranyl always dominates at neutral pH range.
- John Komlos and Peter Jaffé, Princeton University, Princeton, New Jersey, along with EMSL scientist Ravi Kukkadapu and John Zachara, Pacific Northwest National Laboratory, Richland, Washington, collaborated on the effect of oxidation/reduction



**Figure 17.** Jacob Dane visited EMSL for two weeks to help set up the experiment, which included packing the flow cell with various sands.

cycling on microbial Fe(III) reduction of a shale-limestone saprolite sediment containing Fe(III) oxides and Fe(II)/Fe(III) phyllosilicates. The sediment was obtained from a DOE experimental site (Oak Ridge Field Research Center) where in-situ stimulation of dissimilatory iron reduction is being studied as a potential approach to arrest the subsurface migration of mobile radionuclides, e.g. U(VI) and Tc(VIII). In this collaboration, sediments that are reduced and reoxidized in a column study were primarily characterized by cryogenic Mössbauer spectroscopy to monitor changes in iron mineralogy. The purpose of this collaboration was to quantify changes in iron speciation resulting from microbial reduction and subsequent abiotic re-oxidation. Reoxidation of the microbially reduced iron may occur in sediments that experience cycles of oxidation and reduction and can thus impact the fate and extent of contaminant remediation.

- John Weare, University of California, La Jolla, California, collaborated with Eric Bylaska, Pacific Northwest National Laboratory, Richland, Washington, to use ab initio molecular dynamics simulations for modeling the metal ion solvation shell in high-temperature (pressure) electrolyte solutions important in metal ion transport in hydrothermal environments.

## High-Field Magnetic Resonance Facility

- Linan An, Advanced Materials Processing and Analysis Center, University of Central Florida, Orlando, Florida, used the 500-MHz CMX NMR spectrometer to run samples for the “Study of the Structures of Thermally Formed Oxides on Amorphous SiAlCN Ceramics.”
- James Aramini and Gaetano Montelione, Rutgers University, Piscataway, New Jersey, sent samples to be run on the 600-MHz and 800-MHz NMR spectrometers for the study “Structural Genomics of Model Eukaryotic Organisms.”
- Cheryl Arrowsmith, University of Toronto (University Health Network), Toronto, Ontario, Canada, sent samples to be run on the 500-MHz and 750-MHz NMR spectrometers for the study “Structural Proteomics: Annotating the Genome Using 3D Structure.”
- Peter Brzovic and Margaret Daley, University of Washington, Seattle, Washington, used the 600-MHz NMR spectrometer to run samples for the study “NMR Structural Investigations of BRCA1.”
- Brian Cherry, Sandia National Laboratory, Albuquerque, New Mexico, used the 500-MHz wide-bore NMR spectrometer to run samples for the study “Relaxation-NMR-Imaging Investigation of Initiated Polymer Degradation.”
- Andrew Felmy, Pacific Northwest National Laboratory, Richland, Washington, sent samples to be run on the 500-MHz NMR spectrometer for the study “Complexation of Th(IV) by Organic Acids in Aqueous Solution.”
- Leonard Fifield, Pacific Northwest National Laboratory, Richland, Washington, used the 500-MHz CMX NMR spectrometer to run samples for the study “NMR Analysis of Synthesized Organic Compounds for Modification of Nanostructures.”

- Peter Flynn and Sarah Soss, University of Utah, Salt Lake City, Utah, sent samples to be run on the 600-MHz NMR spectrometer for the study “Structure and Dynamics of the 15.5-kD Protein and the 15.5-U4snRNA Complex.”
- Alfred Fuciarelli, Colorado State University, Fort Collins, Colorado, sent samples to be run on the 600-MHz NMR spectrometer for the study “Metabonomics Assessment Following ANIT or Acetaminophen Administration to Male Fischer 344 Rats.”
- James Gibson and Vinodhkumar Raghunathan, University of Washington, Seattle, Washington, used the 500-MHz wide-bore NMR spectrometer to run samples for the “Study of the Binding of SN-15 to Hydroxyapatite Using  $^{15}\text{N}\{^{31}\text{P}\}$  REDOR.”
- Stephen Holbrook, Lawrence Berkeley National Laboratory, Berkeley, California, sent samples to be run on the 500-MHz NMR spectrometer for “Structural Studies of Nudix Hydrolyases from *Bacillus anthracis*, the Bacteria that Produces the Deadly Toxin Anthrax.”
- Jian Zhi Hu, Pacific Northwest National Laboratory, Richland, Washington, used the 750-MHz NMR spectrometer to run samples for the study “Solid-State  $^{183}\text{W}$  MAS NMR at High and Ultra-High Magnetic Fields.”
- Evan Kantrowitz, Merkert Chemistry Center, Chestnut Hill, Massachusetts, sent samples to be run on the 500-MHz and 800-MHz NMR spectrometers for the study “Probing the Mechanism of the Alkaline Phosphatase Reaction by  $^{67}\text{Zn}$  and  $^{25}\text{Mg}$  NMR.”
- Brianna Klein, University of Oregon, Corvallis, Oregon, is working this summer with EMSL researcher Nancy Isern and Shuisong Ni, Pacific Northwest National Laboratory, Richland, Washington, on the purification and structural determination of c-type cytochromes and curl proteins in *Shewanella oneidensis* by X-ray crystallography and nuclear magnetic resonance.
- Thomas Leeper, University of Washington, Seattle, Washington, sent samples to be run on the 600-MHz NMR spectrometer for the study “Structure of Telomerase RNA and Telomeric Proteins.”
- Gregory Marsing, Brigham Young University, Provo, Utah, is working with EMSL researcher Nancy Isern to express and purify c cytochromes from *Shewanella oneidensis* to be used in NMR and crystallographic experiments in protein characterization.
- Bruce McNamara, Pacific Northwest National Laboratory, Richland, Washington, used the 300-MHz CMX NMR spectrometer to run samples for the study “Kinetics of Polyphosphate Decomposition in Heterogeneous Environments.”
- Ryszard Michalczyk and Norma Pawley, Los Alamos National Laboratory, Los Alamos, New Mexico, sent samples to be run on the 600-MHz NMR spectrometer for the study “Structural Studies of the Hyaluronan Receptor CD-44 and CD44-HA Complex.”
- Ponni Rajagopal, University of Washington, Seattle, Washington, used the 800-MHz NMR spectrometer to run samples for the study “Structure and Dynamics of aB57.”

- Raymond Reeves, Washington State University, Pullman, Washington, sent samples to be run on the 500-MHz NMR spectrometer for the study “Structural Biology of the Human High Mobility Group A (HMGA) Proteins: Characterizing the Hub of Nuclear Function.”
- Celine Schneider, University of British Columbia, Vancouver, British Columbia, Canada, used the 750-MHz NMR spectrometer for “Structural Investigations of Solid Materials by High-Resolution Solid-State NMR at Very High Field.”
- Thomas Terwilliger, Los Alamos National Laboratory, Los Alamos, New Mexico, sent samples to be run on the 500-MHz NMR spectrometer for the study “Structural Proteomics of Mycobacterium Tuberculosis.”
- Susan Wallace, University of Vermont, Burlington, Vermont, sent samples to be run on the 600-MHz NMR spectrometer for the study “Interaction of *Escherichia coli* Formamidopyrimidine-DNA Glycosylase (Fpg) with Damaged DNA Containing an 7,8-Dihydro-8-oxoguanine Lesion.”
- Marvin Warner, Pacific Northwest National Laboratory, Richland, Washington, used the 300-MHz CMX NMR spectrometer to run samples for the study “Routine Proton and Carbon-13 NMR Analysis of Functionalized Semiconductor Quantum Dots for Biodetection Studies.”
- John Weil, University of Saskatchewan, Saskatoon, Saskatchewan, Canada, used the electron paramagnetic resonance spectrometer to run samples for the study “Defect Dynamics on Crystalline Quartz.”
- Chin Wu and Christopher Grant, University of California, San Diego, La Jolla, California, used the 900-MHz NMR spectrometer to run samples for the study “Probe Performance Testing at 900 MHz.”

## High Performance Mass Spectrometry Facility

- Diana Bigelow and Colette Sacksteder, Pacific Northwest National Laboratory, Richland, Washington, sent samples to be run on the spectrometers for the study “Proteomics of Membrane Protein Complexes.”
- David Camp, Pacific Northwest National Laboratory, Richland Washington, analyzed various methods of sample preparation for brain samples, and is reviewing the data to determine which method obtained the best results. More sample preparation methods may be performed to further optimize the procedure.
- Matthew Coleman, Lawrence Livermore National Laboratory, Livermore, California, sent samples to be run on the LCQ spectrometers for the study “Identification of Proteins Differentially Expressed in Response IR.”
- Michal Fried, Seattle Biomedical Research Institute, Seattle, Washington, is studying membrane proteins of placental parasites *Plasmodium falciparum* (malaria parasite). In order to identify the membrane proteins, digested protein samples were sent for

analysis on LCQ and Fourier transform ion cyclotron resonance (FTICR) mass spectrometers.

- Mary Lipton, Pacific Northwest National Laboratory, Richland, Washington, ran samples on the LCQ spectrometers for the study of *Deinococcus radiodurans*. In addition, Lipton used the 9.4-tesla FTICR spectrometer to analyze proteomic samples for the *Shewanella* federation that focuses on the characterization of proteins from cells grown in the presence and absence of oxygen. Additionally, under certain conditions, cells produce microfibers and these fibers were also subjected to proteomic analysis.
- Sandra McCutchen-Maloney, Lawrence Livermore National Laboratory, Livermore, California, and Mary Lipton, Pacific Northwest National Laboratory, Richland, Washington, finished qualitative and quantitative analysis for the whole proteome of *Yersina pestis*.
- Curt Scharfe, Stanford University, Stanford, California, sent mitochondrial samples for fractionation using strong cation exchange high-performance liquid chromatography.
- Alfred Spormann, Stanford University, Stanford, California, sent biofilm samples for analysis.
- Arzu Umar, Erasmus Medical Center, Rotterdam, the Netherlands, worked on the study "Identification of Functional Pathways Associated with Clinical Tamoxifen-Resistance in Breast Cancer by Advanced Mass Spectrometry."

## Molecular Science Computing Facility

- Jing Song, Massachusetts Institute of Technology, Cambridge, Massachusetts, gave the seminar "Method of Moments of Coupled-Cluster Equations: A New Tool in Many-Body Quantum Theory."

## Molecular Sciences Software - New User Agreements with NWChem/Ecce

- Academy of Sciences of the Czech Republic, Prague, Czech Republic
- Bayer Polymers, Sarnia, Ontario, Canada
- Claude Bernard University Lyon, Lyon, France
- DSO National Laboratories, Singapore
- East Carolina University, Greenville, North Carolina
- Facultes Universitaires Notre-Dame de la Paix, Namur, Belgium
- Hewlett-Packard Company, Boeblingen, Germany
- Industrial Summit Technology, Parlin, New Jersey
- Institute of Immunology, Third Military Medical University, Chongqing, Peoples Republic of China
- Institute of Solid State Chemistry and Mechanics Chemistry of SB RAS, Novosibirsk, Russia

- Joint Stock Company, SOFT-TEC, Moscow, Russia
- Kennesaw State University, Kennesaw, Georgia
- Korea Institute for Advanced Study, Seoul, Korea
- Massachusetts Institute of Technology, Cambridge, Massachusetts
- Massey University, Auckland, New Zealand
- MV Lomonosov Moscow State University, Moscow, Russia
- NASA Kennedy Space Center, Kennedy Space Center, Florida
- National de Recherche Scientifique, Marseille, France
- National Research Council Canada, Ottawa, Ontario Canada
- National University of La Plata, La Plata, Argentina
- New Jersey Institute of Technology, Newark, New Jersey
- North Carolina State University, Raleigh, North Carolina
- PathScale Inc., Sunnyvale, California
- Russian Academy of Sciences, Moscow, Russia
- Semmelweis University, Budapest, Hungary
- The Dow Chemical Company, Freeport Texas
- Universidad Autonoma San Luis Potosi, San Luis Potosi, Mexico
- Universidad de Santiago de Chile, Santiago, Chile
- Universidad Nacional Autonoma de Mexico, Mexico City, Mexico
- Universidad Nacional de Salta, Buenos Aires, Argentina
- Universidade Federal de Pernambuco, Recife, Brazil
- Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil
- University de Sevilla, Sevilla, Spain
- University of Auckland, Auckland, New Zealand
- University of Bielefeld, Bielefeld, Germany
- University of Calgary, Calgary, Alberta, Canada
- University of California, Los Angeles, Los Angeles, California
- University of Chicago, Chicago, Illinois
- University of Cincinnati, Cincinnati, Ohio
- University of Cologne, Cologne, Germany
- University of Essen, Essen, Germany
- University of Granada, Granada, Spain
- University of Jagiellonski, Krakow, Poland
- University of Louisville, Louisville, Kentucky
- University of North Carolina, Charlotte, North Carolina
- University of Oporto, Oporto, Portugal
- University of Wroclaw, Wroclaw, Poland
- Valdosta State University, Valdosta, Georgia
- Wroclaw University of Technology, Wroclaw, Poland

## Publications

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

Andrews L, B Liang, J Li, and BE Bursten. 2004. "Noble Gas-Uranium Coordination and Intersystem Crossing for the  $\text{CUO}(\text{Ne})_x(\text{Ng})_n$  ( $\text{Ng} = \text{Ar, Kr, Xe}$ ) Complexes in Solid Neon." *New Journal of Chemistry* 28(2):289-294.

Bertram HC, JZ Hu, DN Rommereim, RA Wind, and HJ Andersen. 2004. "Dynamic High-Resolution  $^1\text{H}$  and  $^{31}\text{P}$  NMR Spectroscopy and  $^1\text{H}$   $T_2$  Measurements in Postmortem Rabbit Muscles Using Slow Magic Angle Spinning." *Journal of Agricultural and Food Chemistry* 52(9):2681-2688.

Buchko GW, S Ni, SR Holbrook, and MA Kennedy. 2004. "Solution Structure of Hypothetical Nudix Hydrolase DR0079 from Extremely Radiation-Resistant *Deinococcus radiodurans* Bacterium." *Proteins: Structure, Functions, and Bioinformatics* 56(1):28-39.

Bui JM, K Tai, and AJ McCammon. 2004. "Acetylcholinesterase: Enhanced Fluctuations and Alternative Routes to the Active Site in the Complex with Fasciculin-2." *Journal of the American Chemical Society* 126(23):7198-7205.

Cournia Z, AC Vaiana, GM Ullmann, and JC Smith. 2004. "Derivation of a Molecular Mechanics Force Field for Cholesterol." *Pure and Applied Chemistry* 76(1):189-196.

Daschbach JL, GK Schenter, P Ayotte, RS Smith, and BD Kay. 2004. "Helium Diffusion through  $\text{H}_2\text{O}$  and  $\text{D}_2\text{O}$  Amorphous Ice: Observation of a Lattice Inverse Isotope Effect." *Physical Review Letters* 92(19):198306.

Daughdrill GW, PD Vise, H Zhou, X Yang, WF Yu, ML Tasayco, and DF Lowry. 2004. "Reduced Spectral Density Mapping of a Partially Folded Fragment of *E. coli* Thioredoxin" *Journal of Biomolecular Structure and Dynamics* 21(5):663-670.

Du Y, S Atha, R Hull, JF Groves, IV Lyubinetzky, and DR Baer. 2004. "Focused-Ion-Beam Directed Self-Assembly of  $\text{Cu}_2\text{O}$  Islands on  $\text{SrTiO}_3$  (100)." *Applied Physics Letters* 84(25):5213-5215.

Fifield LS, LR Dalton, RS Addleman, RA Galhotra, MH Engelhard, GE Fryxell, and CL Aardahl. 2004. "Noncovalent Functionalization of Carbon Nanotubes with Molecular Anchors using Supercritical Fluids." *Journal of Physical Chemistry B* 108(25):8737-8741.

Gao F, M Posselt, V Belko, Y Zhang, and WJ Weber. 2004. "Structures and Energetics of Defects: A Comparative Study of 3C- and 4H-SiC." *Nuclear Instruments and Methods in Physics Research Section B, Beam Interactions with Materials and Atoms* 218:74-79.

- Gao W, CM Wang, HQ Wang, VE Henrich, and EI Altman. 2004. "Growth and Surface Structure of Vanadium Oxide on Anatase (001)." *Surface Science* 559(2-3):201-213.
- Gorshkov MV, CD Masselon, EN Nikolaev, HR Udseth, L Pasa-Tolic, and RD Smith. 2004. "Considerations for Electron Capture Dissociation Efficiency in FTICR Mass Spectrometry." *International Journal of Mass Spectrometry* 234(1-3):131-136.
- Goss LM, CD Mortensen, and TA Blake. 2004. "Rotationally Resolved Spectroscopy of the  $\nu_8$  Band of Cis-methyl-nitrite." *Journal of Molecular Spectroscopy* 225(2):182-188.
- Hache JJ, JH Futrell, and J Laskin. 2004. "Relative Proton Affinities from Kinetic Energy Release Distributions for Dissociation of Proton-Bound Dimers: 2. Diamines as a Test Case." *International Journal of Mass Spectrometry* 233(1-3):223-231.
- Hu DH, M Micic, N Klymyshyn, YD Suh, and HP Lu. 2004. "Correlated Topographic and Spectroscopic Imaging by Combined Atomic Force Microscopy and Optical Microscopy." *Journal of Luminescence* 107(1-4):4-12.
- Ivanov I and M Klein. 2004. "First Principles Computational Study of the Active Site of Arginase." *Proteins: Structure, Function, and Genetics* 54(1):1-7.
- Jiang W, CM Wang, WJ Weber, MH Engelhard, and LV Saraf. 2004. "Direct Determination of Volume Changes in Ion-Beam-Irradiated SiC." *Journal of Applied Physics* 95(9):4687-4690.
- Jiang W, WJ Weber, CM Wang, L Wang, and K Sun. 2004. "Experimental Studies of Defects, Implants and Their Processes in Ion-Irradiated Gallium Nitride Single Crystals." In *Defects and Diffusion in Ceramics - an Annual Retrospective - VI, Defect and Diffusion Forum*, vol. 226-228, ed. David J. Fisher, pp. 91-111. Trans Tech Publications, Uetikon-Zurich, Switzerland.
- Jiang W, WJ Weber, V Shutthanandan, L Li, and S Thevuthasan. 2004. "Thermal and Dynamic Responses of Ag Implants in Silicon Carbide." *Nuclear Instruments and Methods in Physics Research Section B, Beam Interactions with Materials and Atoms* 219-220:642-646.
- Kim YJ, S Thevuthasan, TC Droubay, AS Lea, CM Wang, V Shutthanandan, SA Chambers, RP Sears, B Taylor, and B Sinkovic. 2004. "Growth and Properties of Molecular Beam Epitaxially Grown Ferromagnetic Fe-Doped TiO<sub>2</sub> Rutile Films on TiO<sub>2</sub> (110)." *Applied Physics Letters* 84(18):3531-3533.
- Kiran B, X Li, HJ Zhai, LF Cui, and LS Wang. 2004. "[SiAu<sub>4</sub>]: Aurosilane." *Angewandte Chemie International Edition* 43(16):2125-2129.
- Kukkadapu RK, JM Zachara, JK Fredrickson, and DW Kennedy. 2004. "Biotransformation of Two-Line Silica-Ferrihydrite by a Dissimilatory Fe(III)-Reducing Bacterium: Formation of Carbonate Green Rust in the Presence of Phosphate." *Geochimica et Cosmochimica Acta* 68(13):2799-2814.

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- Lugo A, J Fischer, and D Lawson. 2004. "Titanacyclobutadiene: Structure, Properties, and Relative Stability." *Journal of Molecular Structure: THEOCHEM* 674(1-3):139-146.
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- Maki A, TA Blake, RL Sams, J Friehe, J Barber, T Masiello, ETH Chrysostom, JW Nibler, and A Weber. 2004. "Analysis of Some Combination-Overtone Infrared Bands of <sup>32</sup>S<sup>16</sup>O<sub>3</sub>." *Journal of Molecular Spectroscopy* 225(2):109-122.
- Matus MH, J Garza, and M Galvan. 2004. "Basis Set Effects on Frontier Molecular Orbital Energies and Energy Gaps: A Comparative Study Between Plane Waves and Localized Basis Functions in Molecular Systems." *Journal of Chemical Physics* 120(22):10359-10363.
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- Smith RJ, Y Zhang, V Shutthanandan, LJ Bissell, S Thevuthasan, W Jiang, and WJ Weber. 2004. "NRA and ERDA Investigation of Helium Retention in SiC as a Function of

Irradiation and Annealing." *Nuclear Instruments and Methods in Physics Research Section B, Beam Interactions with Materials and Atoms* 219-220:631-635.

Stack AG, CM Eggleston, and MH Engelhard. 2004. "Reaction of Hydroquinone with Hematite I. Study of Adsorption by Electrochemical-Scanning Tunneling Microscopy and X-ray Photoelectron Spectroscopy." *Journal of Colloid and Interface Science* 274(2):433-441.

Stack AG, KM Rosso, DMA Smith, and CM Eggleston. 2004. "Reaction of Hydroquinone with Hematite: II. Calculated Electron Transfer Rates and Comparison to the Reductive Dissolution Rate." *Journal of Colloid and Interface Science* 274(2):442-450.

Stack AG, KM Rosso, DMA Smith, and CM Eggleston. 2004. "Reaction of Hydroquinone with Hematite: II. Calculated Electron-Transfer Rates and Comparison to the Reductive Dissolution Rate." *Journal of Colloid and Interface Science* 274(2):442-450.

Strawn DG, NE Palmer, LJ Furnare, C Goodell, JE Amonette, and RK Kukkadapu. 2004. "Copper Sorption Mechanisms on Smectites." *Clays and Clay Minerals* 52(3):321-333.

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Wang CM, S Azad, S Thevuthasan, V Shutthanandan, DE McCready, and CH Peden. 2004. "Distortion of the Oxygen Sublattice in Pure Cubic-ZrO<sub>2</sub>." *Journal of Materials Research* 19(5):1315-1319.

Wang CM, V Shutthanandan, Y Zhang, LE Thomas, DR Baer, S Thevuthasan, and G Duscher. 2004. "Precipitation of Au Nanoclusters in SrTiO<sub>3</sub> by Ion Implantation." *Journal of Applied Physics* 95(9):5060-5068.

Wang CM, Y Zhang, V Shutthanandan, S Thevuthasan, and G Duscher. 2004. "Microstructure of Precipitated Au Nanoclusters in TiO<sub>2</sub>." *Journal of Applied Physics* 95(12):8185-8193.

Wang X, L Andrews, J Li, and BE Bursten. 2004. "Significant Interactions Between Uranium and Noble-Gas Atoms: Coordination of the UO<sub>2</sub><sup>+</sup> Cation by Ne, Ar, Kr, and Xe Atoms." *Angewandte Chemie International Edition* 43(19):2554-2557.

Waters T, XB Wang, X Yang, L Zhang, RAJ O'Hair, LS Wang, and AG Wedd. 2004. "Photoelectron Spectroscopy of the Doubly-Charged Anions [M<sup>IVO</sup>(mnt)<sub>2</sub>]<sup>2-</sup> (M = Mo, W; mnt = S<sub>2</sub>C<sub>2</sub>(CN)<sub>2</sub><sup>2-</sup>): Access to the Ground and Excited States of the [MVO(mnt)<sub>2</sub>]<sup>-</sup> Anion." *Journal of the American Chemical Society* 126(16):5119-5129.

Wu K, J Li, and C Lin. 2004. "Remarkable Second-Order Optical Nonlinearity of Nano-Sized Au<sub>20</sub> Cluster: A TDDFT Study." *Chemical Physics Letters* 388(4-6):353-357.

Yantasee W, Y Lin, GE Fryxell, and Z Wang. 2004. "Carbon Paste Electrode Modified with Carbamoylphosphonic Acid Functionalized Mesoporous Silica: A New Mercury-Free Sensor for Uranium Detection." *Electroanalysis* 16(10):870-873.

Zhai HJ, AN Alexandrova, KA Birch, AI Boldyrev and LS Wang. 2003. "Hepta- and Octacoordinate Boron in Molecular Wheels of Eight- and Nine-Atom Boron Clusters: Observation and Confirmation." *Angewandte Chemie-International Edition* 42(48): 6004-6008

Zhai HJ, LS Wang, P Jena, GL Gutsev, and CW Bauschlicher. 2004. "Competition Between Linear and Cyclic Structures in Monochromium Carbide Clusters  $\text{CrC}_n^-$  and  $\text{CrC}_n$  ( $n=2-8$ ): A Photoelectron Spectroscopy and Density Functional Study." *Journal of Chemical Physics* 120(19):8996-9008.

Zhang Y and WJ Weber. 2004. "Studies of Electronic Stopping Powers Using Time of Flight Spectrometry." *Nuclear Instruments and Methods in Physics Research Section B, Beam Interactions with Materials and Atoms* 219-220:256-262.

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Zhang Y, WJ Weber, W Jiang, V Shutthanandan, S Thevuthasan, M Janson, and A Hallen. 2004. "Annealing Behavior of Al-Implantation-Induced Disorder in 4H-SiC." *Nuclear Instruments and Methods in Physics Research Section B, Beam Interactions with Materials and Atoms* 219-220:647-651.

## Presentations

Although not an inclusive list, the following illustrates the variety of topics presented by staff members and users at meetings and events. EMSL does not typically collect presentation information from users external to the laboratory.

Alexander ML, JS Young, and PF Martin. 2004. "Gas Hydrate Formation and Dissociation in the Environmental Scanning Electron Microscope." Presented by B. Peter McGrail at the Goldschmidt Geochemistry Conference, Copenhagen, Denmark, on June 8, 2004.

Ayotte P, JL Daschbach, Z Dohnalek, GA Kimmel, KP Stevenson, GR Teeter, RS Smith, and BD Kay. 2004. "Using Nanoscale Amorphous Films to Study Processes in Supercooled Liquid Water and Aqueous Solutions." Presented by Bruce D. Kay (Invited Speaker) at Argonne National Laboratory, Argonne, Illinois, on May 3, 2004.

Baran M, JM Aramini, J Huang, and G Montelione. 2004. "NESG Rossetta Stones Unturned." Presented by James Aramini at EMSL 2004, Richland, Washington, on June 14, 2004.

Bhattacharya A, Z Wunderlich, R Tejero, and G Montelione. 2004. "Protein Structure Validation Software and its Applications in Evaluating Structures Generated by Structural Genomics and Homology Modeling." Presented by Gaetano Montelione at EMSL 2004, Richland, Washington, on June 14, 2004.

Buchko GW, K McAteer, SS Wallace, and MA Kennedy. 2004. "NMR Evidence for Conformational Changes to *Escherichia coli* Formamidopyrimidine-DNA Glycosylase (Fpg) upon Binding DNA Containing an Abasic Site Analogue." Presented by Garry Buchko at the VIIIth International Workshop on Radiation Damage to DNA, Banff, Alberta, Canada, on May 26, 2004.

Buchko GW, K McAteer, SS Wallace, and MA Kennedy. 2004. "NMR Studies of DNA Binding Interactions in *Escherichia coli* Formamidopyrimidine-DNA Glycosylase (MutM): A Dynamic Description of the DNA/Protein Interface." Presented by Garry Buchko at EMSL 2004, Richland, Washington, on June 14, 2004.

Buchko GW, S Ni, SR Holbrook, and MA Kennedy. 2004. "Structural Characterization of the NUDIX Hydrolyase DR0079 from the Extremely Radiation-Resistant Bacterium *Deinococcus radiodurans*." Presented by Garry W. Buchko at EMSL 2004, Richland, Washington, on June 14, 2004.

Cherry BR. 2004. "Relaxation Nuclear Magnetic Resonance Imaging (R-NMRI) of Heterogeneous Polymer Aging." Presented by Brian Cherry at EMSL 2004, Richland, Washington, on June 14, 2004.

Choowongkomon K. 2004. "Solution NMR Spectroscopy for the Structural Characterization of Integral TB membrane Proteins and Juxtamembrane EGFR." Presented by Kiattawee Choowongkomon at EMSL 2004, Richland, Washington, on June 14, 2004.

Cooper DC, MA Plummer, DT Fox, RK Kukkadapu, and LC Hull. 2004. "Uranium and Tritium Transport in Vadose Zone Sediments." Presented by D. Craig Cooper at the 41st Clay Minerals Society Meeting, Richland, Washington, on June 21, 2004.

Cort JR, A Yee, B Wu, JM Aramini, TA Ramelot, CH Arrowsmith, G Montelione, and MA Kennedy. 2004. "Protein Structures from the Northeast Structural Genomics Consortium Determined Using NMR Data Collected at EMSL." Presented by JohnCort at EMSL 2004, Richland, Washington, on June 14, 2004.

Cort JR, R Xiao, Y Chiang, G Montelione, and MA Kennedy. 2004. "NMR Structure and Enzyme Mechanism of 5,10-methenyltetrahydrofolate Synthetase from *Aquifex aeolicus*." Presented by John Cort at EMSL 2004, Richland, Washington, on June 14, 2004.

Cotten M. 2004. "Investigating Molecular Recognition and Biological Function at Interfaces Using Piscidins, Antimicrobial Peptides from Fish." Presented by Myriam Cotten at EMSL 2004, Richland, Washington, on June 14, 2004.

Cowley DE. 2004. "High-Performance Technical Computing at Pacific Northwest National Laboratory." Presented by Dave Cowley (invited speaker) at the National Laboratories Information Technology Summit, Jackson Hole, Wyoming, on June 21, 2004.

Crosson GS, KT Mueller, S Choi, J Chorover, and MK Amistadi. 2004. "High-Field Solid State Nuclear Magnetic Resonance Studies of Clay and Feldspathoid Systems: Progress and Future Directions." Presented by Garry Crosson at EMSL 2004, Richland, Washington, on June 14, 2004.

Daley ME, P Brzovic, AV Lissounov, T Ohta, and RE Klevit. 2004. "Structural and Functional Consequences of a Cancer-Associated Mutation in BRCA1 ." Presented by Margaret Daley at EMSL 2004, Richland, Washington, on June 14, 2004.

Ding YR, KK Hixson, S Ciufo, A Stanley, A Esteve-Nunez, WC Lin, JB Burns, and DR Lovley. 2004. "Proteomic Investigation of c-type of Cytochromes in *Geobacter sulfurreducens*." Presented by Kim Hixson (Invited Speaker) at the American Society for Microbiology Conference, New Orleans, Louisiana, on May 23, 2004.

Droubay TC, J Osterwalder, SM Heald, S Thevuthasan, V Shutthanandan, CM Wang, and SA Chambers. 2004. "OPA-MBE Growth and Properties of Cr-Doped TiO<sub>2</sub> Anatase." Presented by Tim Droubay at the Surface Analysis 2004/Pacific Northwest Chapter of the American Vacuum Society 2004, Richland, Washington, on June 16, 2004.

Fan D. 2004. "High-Field NMR Spectroscopy and Molecular Basis of the Pathophysiology of Atherosclerosis." Presented by Daping Fan at EMSL 2004, Richland, Washington, on June 14, 2004.

Felix EJ. 2004. "HPCS2: The Success of the IA64 Cluster." Presented by Evan Felix (Invited Speaker) at the Gelato Strategy Council Meeting, Urbana, Illinois, on May 26, 2004.

Foster NS, TJ Johnson, SE Thompson, NB Valentine, and JE Amonette. 2004. "FTIR Spectroscopy for the Statistical Identification of Vegetative and Sporulated Bacteria." Presented by Nancy S. Foster at the American Chemical Society Northwest Regional Meeting, Logan, Utah, on June 8, 2004.

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